THE DETERMINATION OF OPTIMUM NOZZLE PROFILES TO DELAY CHEMICALLY FROZEN FLOW IN THE EXPANSION OF HIGH TEMPERATURE GAS MIXTURES

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by

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ABSTRACT

An approximate method is presented which yields the supersonic nozzle profile necessary to keep an expanding high temperature gas mixture approximately in chemical equilibrium. From equilibrium calculations for given chamber conditions, the freeze area ratio is determined by use of a modified Bray criterion. A plot of area ratio versus a function of nozzle geometry defines a limiting nozzle angle beyond which freezing is forecast to occur. This permits an expansion angle at each area ratio to be chosen to keep the flow near equilibrium. The effectiveness of the resulting nozzle profile is evaluated by comparing exact calculations with equilibrium calculations. Contouring is shown to be effective for small nozzles when a correction factor is applied. The hydrogen-oxygen system is used as an example.

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TABLE OF SYMBOLS

A	Area (ft^2)
B	Defined in equation (1)
EM	Equilibrium margin--See Fig. 1
ϵ	Area ratio (A/A^*)
I_{sp}	Specific Impulse (lb_f-sec/lb)
k_b	Backward rate constant
k_f	Forward rate constant
L	Length (ft)
M	Third body
$\overline{m}$	Mean molecular weight
$\dot{m}$	Mass flow rate (lb_m/sec)
n	Molar density (lb-mol/ft^3)
P_c	Chamber pressure
r	Radius (ft)
R'	Recombination rate
R''	Dissociation rate
σ	Concentration (lb-mol/lb)
v	Velocity (ft/sec)
X	Mole fraction
$(\ )^*$	Throat variable

1. Introduction.

During the last decade a marked increase of interest in rocket design and performance prediction has occurred. Payloads for space exploration missions often differ greatly from those of a military nature, but the vehicles involved have a major common factor which is the rocket engine. Methods of propulsion currently under investigation for the future include ion, magnetoplasma, and nuclear fission; however, the primary type today is the chemical rocket engine.

The idea of jet propulsion is old. In the chemical rocket, potential chemical energy of the fuel and oxidizer is converted into thermal energy in the combustion chamber. A convergent-divergent de Laval nozzle then accelerates the gas stream from subsonic to supersonic velocity. This converts the thermal energy and pressure potential energy of the nearly stagnant, hot gas ahead of the nozzle into the kinetic energy of the supersonic stream which emerges with lower temperature and pressure. A reaction is imparted which is directly related to the time rate of change of the momentum of the ejected matter.

At the high temperatures encountered in modern combustion chambers, a large part of the chemical energy released may be used in breaking chemical bonds to produce simpler species (dissociation). As the temperature and pressure decrease during expansion, recombination of the simpler species occurs with a resulting release of chemically bound energy to the gas flow. A significant portion of the chemical energy is not available for conversion to kinetic energy unless reassociation of the dissociated combustion products

occur. Thus, the thrust produced by any propulsive system in which combustion products are expanded through a nozzle will be reduced if the recombination process cannot occur rapidly enough to remain in equilibrium.

In a rocket nozzle the elementary reactions between the dissociated combustion products seldom proceed at rates which are sufficient to maintain true chemical equilibrium throughout the nozzle expansion [16]*. For a hypersonic ramjet, calculations indicate net thrusts which are attractively high if equilibrium is maintained, but which approach zero around mach numbers of ten or eleven if the combustion products are frozen, i.e., constant composition [3].

To facilitate further discussion, the following descriptions of flows are given:

Frozen: The chemical reaction rates are zero with composition invariant. Typical non-reacting flows come under this classification.

Equilibrium: The chemical reaction rates are infinite, and composition of the gas adjusts instantaneously to changes in temperature and pressure.

Exact: The chemical reaction rates are finite. A finite time is required for the composition of the gas to adjust to the changes dictated by the pressure and temperature variations in the nozzle.

* Numbers in brackets indicate references on page 30.

Near-equilibrium flow and near-frozen flow imply a small deviation from the artificial cases of zero or infinite reaction rates without an appreciable change in the resulting performance prediction. Equilibrium flow yields maximum performance while frozen flow yields minimum performance.

Consider the following typical three-body reaction:

$$A + B + M \underset{R''}{\overset{R'}{\rightleftharpoons}} AB + M$$

where M is a third body which removes the energy during recombination, and R' and R" are the rates of the reaction in the forward (recombination) and backward (dissociation) directions respectively. In the combustion chamber, the reaction would move to the left. At lower temperatures and pressures, the equilibrium composition would shift toward the formation of AB.

If, however, the reaction rates are not fast enough to maintain the equilibrium conditions, recombination will lag. The gas leaving the nozzle will have some dissociated products which have not contributed to the kinetic energy of the flow. A reduction in thrust will occur if the recombination process does not occur rapidly enough to remain in equilibrium.

It is assumed that the working fluid is a mixture of ideal gases; that the flow is steady, adiabatic, and quasi-one-dimensional; and that the effects of diffusion, heat conduction, and viscosity are negligible. Equilibrium flow calculations involve the simultaneous solution of the algebraic equations for conservation of mass, energy, momentum, and species plus the equation of state. Frozen flow calculations are the same except that the species composition is constant during the flow. These two types of calculations

present no particular difficulties. Many computer programs have been written to yield gas dynamic and thermodynamic data at selected stations [4, 5, 6].

For an exact flow, though, the problem is more complex. Sarli, et al., [16], summarizes the difficulties. The calculations require the simultaneous solution of the mass, momentum, and energy conservation equations; state and mixture enthalpy equations; kinetic differential equations for the finite rate of production of molecular species; and atomic continuity equations for all atoms present. The equations used in the exact solution are given in Appendix I. Again the assumptions are that the flow is one-dimensional, inviscid, and adiabatic, with negligible diffusion. The simultaneous solution of the above equations requires numerical techniques; hence, a digital computer is desirable [9, 10, 16].

Three basic problems exist, however, regarding these exact calculations [16]. These are: 1. The numerical integration of the equations, when near-equilibrium conditions exist in the flow, is relatively slow and potentially inaccurate; 2. It is necessary to specify the detailed mechanism and individual rates for the reactions taking place; 3. The cost of the computer time involved prohibits casual investigations of complex, reacting flows.

Today's space ventures require thrust prediction and/or weight minimization such that a design based solely on a frozen flow calculation or an equilibrium flow calculation would be unacceptable. This does not mean that equilibrium and frozen calculations are to be abandoned. In view of the computational problems mentioned above that exist with the exact solutions, a method of establishing guidelines for the design of rocket nozzles is desir-

able which utilizes approximate methods.

One of the first to investigate a modified equilibrium/frozen calculation to predict actual performance was Penner [12]. Criteria were established which, in some instances, permitted a nozzle flow to be classified as near-equilibrium or near-frozen. Thus, for a given set of conditions, a reasonable prediction of performance could be given without encountering the complexities of an exact calculation. Reichenbach [15] proposed an iterative procedure for the solution of nozzle flow problems. Agreement with exact calculations was generally good. Several investigators [1, 11] have considered the design of an optimum nozzle.

Another early investigator in this area was Bray [2, 3]. His work has received considerable attention since its first presentation in 1958. Many of the current papers in the field of nozzle flow with chemical reactions utilize his concepts.

The Bray criterion is an approximate procedure for prediciting where a reaction has departed significantly from equilibrium in a reacting nozzle flow. This prediction is made by determining the point at which the forward rate of reaction, R', becomes of the same order as the rate required to maintain equilibrium. The flow upstream is considered in equilibrium, while that downstream is considered frozen (invariant in chemical composition). While Bray's original work dealt with a single reaction system, later investigators [3, 7, 8, 16] extended the principle to include multiple reaction systems.

An important point to consider is the effect of nozzle size and geometry on performance. Penner points out [12] that the reaction time must be small

compared with the residence time to achieve near-equilibrium. Hence, for small nozzles (short residence time) it is difficult to achieve near-equilibrium flows.

After the above mentioned calculations are completed, it is then apparent whether or not the boundary configuration chosen (nozzle geometry) is likely to give the desired performance, i.e. thrust and specific impulse. A series of computations using different nozzle geometries would eventually yield a suitable nozzle design, but this would not be economical in terms of expense and labor.

Kushida [8] and Koppang, et al., [7] presented a method utilizing the Bray criterion to determine the freeze point for a given nozzle. Reichenbach [14] suggested to this investigator that a reverse approach might be plausible. Since an estimate is available from Bray's criterion for the location of a freeze point as a function of area ratio, a nozzle designed to avoid the conditions that lead to freezing of the flow could approach the optimum performance for a given system. A further advantage would be the relatively simple calculations involved which use equilibrium data.

An analysis of this approach was undertaken in this paper. The system investigated was hydrogen and oxygen. To compare and evaluate the results, an exact calculation of the system was performed.

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computer facility for their cooperation and assistance in adapting the computer programs to the Control Data Corporation 1604 system.

2. Analysis.

A common form [7, 8, 16, 17] for Bray's sudden freezing criterion is the following semi-theoretical relaxation parameter:

$$B = \frac{\text{Equilibrium rate of change of species } j}{\text{Rate of the recombination reaction } R_j} \tag{1}$$

Thus, B relates equilibrium composition change to the exact composition change. If the ratio is large, the reaction would be near-frozen; if the ratio is small, the reaction would be near-equilibrium. It is generally agreed that the freeze point is determined when B is near unity [1, 7, 8].

For a three-body recombination reaction as shown in equation (1), the recombination rate, R', and the dissociation rate, R", are given by [7]:

$$R' = k_f n^3 X_A X_B X_M \tag{2}$$

$$R'' = k_b n^2 X_{AB} X_M \tag{3}$$

where k_f and k_b are the reaction rate constants (assumed to be a function of temperature only); n is the molar density of the gaseous mixture; and X_A, X_B, X_{AB}, and X_M are the mole fractions of the respective atoms and molecules.

It has been shown [7, 8] that the bimolecular atom transfer, or metathetic reactions, are an order of magnitude faster than the three-body reactions. Also, the energy released by the metathetic reactions is small compared with the three-body reactions. Consequently, the metathetic reactions are assumed to be in equilibrium for this study. Equation (4) is a typical metathetic reaction.

$$OH + O \underset{R''}{\overset{R'}{\rightleftharpoons}} H + O_2 \qquad (4)$$

The main reactions to consider in the hydrogen-oxygen system are the following [7, 8, 16]:

$$\begin{aligned} &1. \quad H + H + M = H_2 + M \\ &2. \quad O + O + M = O_2 + M \\ &3. \quad H + O + M = OH + M \\ &4. \quad OH + H + M = H_2O + M \end{aligned} \qquad (5)$$

It has been found [7] that a system of this type is dependent on the dissappearance of hydrogen to determine the freeze point. As shown by Kushida [8] and Koppang, et al. [7], the net rate of disappearance of monatomic hydrogen is given by:

$$-\bar{m}n \frac{d(X_H/\bar{m})}{dt} = R'_1 + R'_3 + R'_4 - R''_1 - R''_3 - R''_4 \qquad (6)$$

where: $\bar{m}$ is the mean molecular weight, and the subscripts on R refer to the reactions in equation (5).

The reaction rates are determined as shown by Penner [12].

$$\begin{aligned} R'_1 &= k_1(2)(nX_H)(nX_H)(nX_M) = 2\,k_1 n^3 X_H^2 X_M \\ R'_3 &= k_3(1)(nX_H)(nX_O)(nX_M) = k_3 n^3 X_H X_O X_M \\ R'_4 &= k_4(1)(nX_{OH})(nX_H)(nX_M) = k_4 n^3 X_{OH} X_H X_M \end{aligned} \qquad (7)$$

Since X_M is the mole fraction of any third body, it is unity. Rewriting equation (7):

$$R'_1 = 2\,k_1\,n^3\,X_H^{\,2} \qquad (8)$$

$$R'_3 = k_3 n^3 X_H X_O$$

$$R'_4 = k_4 n^3 X_{OH} X_H$$

To obtain the expression for B as shown in equation (1), the equilibrium rate of change of hydrogen concentration is divided by the rate of the recombination reactions for hydrogen. It should be noted that R' represents the rate of recombination and R" represents the rate of dissociation.

$$B = \frac{\bar{m} n\, d(X_H/\bar{m})/dt}{R'_1 + R'_3 + R'_4}$$

$$= \frac{\bar{m} n\, d(X_H/\bar{m})/dt}{2\, k_1 n^3 X_H{}^2 + k_3 n^3 X_H X_O + k_4 n^3 X_{OH} X_H}$$

$$= \frac{\bar{m}\, d(X_H/\bar{m})/dt}{X_H n^2 (2k_1 X_H + k_3 X_O + k_4 X_{OH})} \qquad (9)$$

$$B = \frac{d[\ln (X_H/\bar{m})]/dt}{n^2 (2\, k_1 X_H + k_3 X_O + k_4 X_{OH})}$$

Introducing $v = dL/dt$ and dividing both sides by $d(\epsilon)$ where $\epsilon = A/A^*$ (area divided by the throat area):

$$\frac{B}{d\epsilon} = \frac{v\, d[\ln (X_H/\bar{m})]\, v/dL}{n^2 (2\, k_1 X_H + k_3 X_O + k_4 X_{OH})\, d\epsilon}$$

Rearranging:

$$\frac{B}{d\epsilon/dL} = \frac{v\, d[\ln (X_H/m)]/d\epsilon}{n^2\, (2\, k_1 X_H + k_3 X_O + k_4 X_{OH})} \qquad (10)$$

The right side of equation (10) can be calculated using equilibrium data for a given system. The rate constants, k_f and k_b, are assumed to be functions of temperature only. By plotting the right side of equation (10) versus area ratio, a means of determining the freeze point is provided. For every freeze area ratio, there is a corresponding value for $B/(d\epsilon/dL)$. (Curve A, Fig. 1)

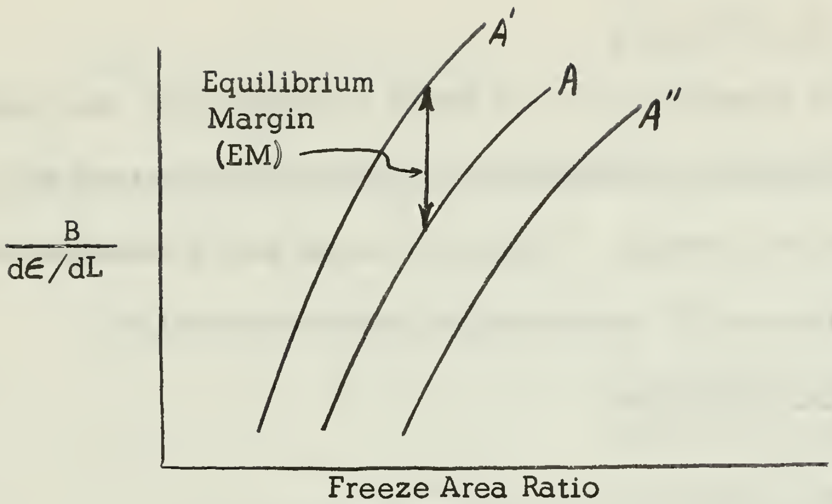

Figure 1: Freeze Point Location

Since B is assumed to be constant and equal to unity, it is thus seen that the local value of $d\epsilon/dL$ determines the freeze point. Therefore, if the nozzle is designed such that $d\epsilon/dL$ is less than the local value for each freeze area ratio (Curve A'), the flow should remain in near-equilibrium. If the nozzle is designed such that $d\epsilon/dL$ is greater than the local value for each freeze area ratio (Curve A"), the flow should become near-frozen.

The vertical distance between Curve A and Curve A' is arbitrary and not necessarily constant. It is important to note, though, that a small displacement from Curve A possibly would not yield near-equilibrium flow because of the inherent inaccuracies introduced by the assumptions. A large displacement would increase the nozzle length because of the slower expansion to a given area ratio. This displacement will be referred to as the equilibrium margin (EM). Since the curves in Fig. 1 are usually plotted on semi-logarithmic paper, the constant displacement EM becomes a multipler to the basic curve.

The information available from Fig 1 thus provides a guide for nozzle design which incorporates the effects of chemistry.

3. Procedure.

The first step necessary in determining a nozzle profile is the calculation of the right side of equation (10). All of the values used are those obtained from equilibrium flow with the exception of the rate constants. The rate constants, however, may be assumed to be functions of the equilibrium temperature at each point in the nozzle. Since equilibrium flow is independent of the nozzle geometry, the same values calculated for one system (chamber conditions, O/F ratio, and reactants) can be used in the study of any nozzle geometry, regardless of size.

Values for $d\left[\ln(X_H/\bar{m})\right]/d\epsilon$ may be obtained graphically or by analytical methods once X_H and $\bar{m}$ are known for different area ratios. This permits the right side of equation (10) to be calculated and plotted versus freeze area ratio, and now represents $B/(d\epsilon/dL)$ as a function of freeze area ratio.

To convert this into an axisymmetric nozzle profile, the following geometric relationship may be used [7] :

$$\frac{d\epsilon}{dL} = \frac{d(r/r^*)^2}{dL} = \frac{2r}{r^*}\,\frac{d(r/r^*)}{dL} \qquad (11)$$

and $dr/dL = \tan\theta$ (12)

where θ is the half-angle of the nozzle. Then

$$\frac{d\epsilon}{dL} = \frac{2r}{r^*}\,\frac{\tan\theta}{r^*} = \frac{2\sqrt{\epsilon}\,\tan\theta}{r^*} \qquad (13)$$

or $\tan\theta = \dfrac{d\epsilon}{dL}\,\dfrac{r^*}{2\sqrt{\epsilon}}$ (14)

Since $d\epsilon/dL$ is available from the previous calculation of $B/(d\epsilon/dL)$, equation (14) provides local values of θ for every freeze area ratio. It should

be noted that nozzle size is now present in that equation (14) involves the throat radius, r^*.

The half-angle, θ, is conveniently calculated by obtaining an expression for $B/(d\epsilon/dL)$ as a function of area ratio. If B is assumed to be unity, then a polynomial form for $d\epsilon/dL$ is

$$dL/d\epsilon = b_o + b_1\epsilon + b_2\epsilon^2 + b_3\epsilon^3 + b_4\epsilon^4 \tag{15}$$

where b_o, b_1, etc. are appropriate coefficients.

Equation (15) may be integrated with the boundary conditions that $\epsilon = 1.0$ at $L = 0$.

$$L = b_o\epsilon + \frac{b_1\epsilon^2}{2} + \frac{b_2\epsilon^3}{3} + \frac{b_3\epsilon^4}{4} + \frac{b_4\epsilon^5}{5} - (b_o + b_1 + b_2 + b_3 + b_4) \tag{16}$$

Using equations (14), (15), and (16), the half-angle and nozzle length may be calculated for each freeze area ratio. Since the throat radius has been set, the throat area is known. With the area ratio and the throat area, the local area and thus the nozzle radius are determined. If an equilibrium margin is desired, it must be applied to both equations (15) and (16).

Special provisions must be made near the nozzle throat. The right side of equation (10) becomes very small as the area ratio approaches one. Thus, $d\epsilon/dL$ is large and, as equation (14) shows, the half-angle approaches 90 degrees. This is unacceptable from a gas dynamics approach. While this difficulty is not the concern of this study, it should be recognized as an area requiring special handling.

Some method of fairing in the profile near the throat must be used until the area ratio permits the contour determined by equation (14). When this point in the nozzle is reached, the values of L must be adjusted since they

no longer conform to the calculated contour. This correction is a constant shift of the L values. As long as the faired section near the throat has local half-angles less than that given by equation (14), the flow should remain in near-equilibrium. Since the allowable half-angles in this region are large, no particular difficulty is encountered.

At large area ratios, θ becomes very small. Thus, it is usually desirable to terminate the contouring after the majority of the benefits of increased recombination have been realized. Further expansion may be accomplished at more rapid rates with consequent near-frozen flow.

4. Results and Discussion.

A study of a particular system was performed to check the validity of the proposed method of nozzle design. The hydrogen-oxygen system was chosen because of its relative simplicity and limited number of combustion products. A chamber pressure of 300 psia and an oxidizer-to-fuel weight ratio of six was chosen as representative of current combustion conditions.

Equilibrium and frozen values for the above mentioned conditions were computed with the aid of a computer program written by Gordon and Zelznik [5, 6]. Tabulated results may be found in Appendix II. The computer program was written for the IBM 7090 system. Since the computer at the Naval Postgraduate School is a CDC 1604, several modifications due to system differences were necessary so that the equilibrium calculations could be made. The basic program was unchanged.

A least-squares curve fitting routine was used to obtain a third order polynomial relating $\ln(X_H/\bar{m})$ and area ratio.

$$\ln (X_H/\bar{m}) = a_O + a_1\epsilon + a_2\epsilon^2 + a_3\epsilon^3 \qquad (17)$$

where: $a_O = 5.22823$

$$a_1 = 5.22515 \times 10^{-1}$$

$$a_2 = -4.27257 \times 10^{-2}$$

$$a_3 = 1.61956 \times 10^{-3}$$

$$\text{Then } d\left[\ln (X_H/\bar{m})\right]/d\epsilon = a_1 + 2a_2\epsilon + 3a_3\epsilon^2 \qquad (18)$$

The rate constants k_1, k_3, and k_4 were calculated from the following relationship:

$$k = DT^E \exp (F/T) \qquad (19)$$

where T is the local equilibrium temperature and D, E, and F are constants listed in Table I [18].

TABLE I

REACTION RATE CONSTANTS

Reaction	D	E	F
1	2.3555×10^{17}	-1.4998	-1493
3	5.5000×10^{11}	0.0000	-10000
4	1.7268×10^{16}	-1.0900	5375

Using equation (18), equation (19), and the equilibrium values, the right side of equation (10) was then calculated. The results are given in Table II. As seen from equation (10), these values also represent $B/(d\epsilon/dL)$. Thus, the locus of points shown in Fig. 2 (EM = 1.0) defines the hypothesized boundary below which departures from near-equilibrium flow probably occur. The values for EM = 1.5 were obtained by multiplying the basic curve (EM = 1.0) by 1.5. The choice of 1.5 was arbitrary. In view of the possible inaccuracies introduced by the simplifying assumptions made in

the formulation of the problem, it was assumed a factor of approximately EM = 1.5 was sufficient. It should be remembered that EM = 1.0 represents the point where, theoretically, the flow is just able to maintain near-equilibrium. A large value for EM would result in a long nozzle since the expansion would be slower. Also, an additional important aspect of this design method is to determine the maximum rate of expansion which may be used and still maintain near-equilibrium conditions.

A polynomial of $B/(d\epsilon/dL)$ as a function of area ratio was obtained with a curve-fit routine which resulted in the following coefficients:

$$b_o = 9.28458 \times 10^{-3}$$

$$b_1 = -2.39544 \times 10^{-2}$$

$$b_2 = 1.34259 \times 10^{-2}$$

$$b_3 = 3.95404 \times 10^{-3}$$

$$b_4 = -3.83076 \times 10^{-5}$$

Equation (14) was used to determine the maximum expansion angle that the flow could tolerate without departing from near-equilibrium. These values are shown in Table III. It should be noted that small area ratios yield large values for θ.

Calculations were performed with nozzle throat radii of 2.0 inches, 0.96 inches, and 0.12 inches. These different size nozzles were identified as Run 1, Run 2, and Run 3. A designation was added to each run to indicate whether the nozzle was a straight conical expansion (S), a contoured expansion (C), or a contour expansion with EM = 1.5 (CM). For example, the run with the two-inch throat that had a contoured expansion with EM = 1.0 was

designated Run 1-C.

A maximum of 45 degrees was used for all runs except Run 3-CM where θ was limited to 30 degrees. In all cases, a circular arc of radius 0.4 times the throat radius was used to fair in the profile near the throat [13]. A linear section was used on the contoured nozzles (1-C, 1-CM, 2-C, and 3-CM) which was carried to the point where the area ratio indicated that the contoured expansion angle as shown in Table III was permissable. The straight conical expansions were all at 15 degrees. See Table IV for a further description of the nozzles. Figs. 3, 4, 5, and 6 show the profiles used. Tables V to XI give the nozzle geometry for each run.

Exact calculations for all seven runs were made with the computer program written by Zupnik, Nilson, and Sarli [18]. As with the equilibrium computer program, certain system modifications were necessary to convert from the IBM 7090 to the CDC 1604. Tabulated values obtained in these calculations are shown in Appendix III.

The benefits of maintaining equilibrium flow can be seen from Fig. 7. Even at the throat, the specific impulse difference is five secs. As the expansion continues, the difference increases to 20 secs at an area ratio of 40.

Figs. 8, 9, and 10 illustrate the effect of contouring on performance for the different nozzle sizes. The contour is most effective on run 3-CM and is insignificant on run 2-C. The apparent explanation for run 2-C is that this run is not modified. That is, it does not have the equilibrium margin that runs 1-CM and 3-CM have. Also, a small nozzle is subject to earlier freezing than is a large one. This is due to the smaller residence time in a

small nozzle which gives less time for the recombination reactions to take place.

Runs 2-C and 2-S illustrate the effect of any contour on nozzle length. Fig. 12 shows that a specific impulse of 365 lb-sec/lb may be obtained with a 0.10 foot nozzle for the contoured nozzle. The straight conical nozzle, though, needs 0.17 feet for the same performance. For a given length of 0.08 feet, the specific impulse difference is 28 secs.

The most significant result is that shown by the small nozzle. Even at relatively small area ratios the effect of contouring is evident. At an area ratio of 40, the difference in specific impulse is six secs. While this is not a large percentage increase, the effect over a long period would be appreciable. Thus, long burn times would require less fuel for the same total performance. Where weight is a critical factor, contouring is particularly advantageous. For a hotter system such as hydrogen-fluorine, the percentage increase in performance is expected to be more significant.

The variation of hydrogen concentration is given in Figs. 13, 14, and 15. The equilibrium value is seen to decrease uniformly with area ratio. In each nozzle size, though, the exact concentrations show a leveling off which indicates a departure from equilibrium. For the conical nozzles the change is gradual, but it occurs where the allowable expansion angle is exceeded (15 degrees). All of the contoured nozzles shown a marked "knee" in the hydrogen concentration when the contouring is stopped (about an area ratio of 4.0). Thus, the effect of contouring a nozzle to delay departure from equilibrium appears to be significant.

Each of the figures illustrating hydrogen concentration shows a gradual deviation from the equilibrium values at small area ratios. It is felt that this is the effect of finite rate constants and not due to inaccuracies in the exact calculations. When large rate constants ($k = 10^{20}$) were used, the exact values essentially duplicated those of the equilibrium calculations. Also, when small rate constants were used ($k = 100$), the concentrations were invariant indicating frozen or non-reacting flow.

The temperature distribution during expansion is given in Fig. 16. Run 3-CM has larger temperatures than Run 3-S. This indicates that more recombination is occurring in the contoured nozzle than in the straight conical nozzle.

As mentioned above, the amount of equilibrium margin used was arbitrarily chosen as 1.5. Further investigation should indicate an optimum factor for EM. A further improvement would be to correlate the increase in weight due to a longer nozzle with the increased performance.

The approach used in this thesis was formulated with hydrogen disappearance as the indication of the freeze point and subsequent deviation from near-equilibrium conditions. Further study might show that other species such as OH or monatomic oxygen give better results. Possibly a combination of species could be used. Sarli, et al. [16] investigated this modified approach in determining the freeze point for multiple reactions. This could serve as a significant refinement to the basic method of determining optimum nozzle contours.

5. Conclusions.

Optimum contouring of a nozzle by use of a sudden freeze criterion results in a delay of the departure from near-equilibrium flow and an increase in performance. This is relatively more effective with smaller nozzles where recombination normally lags because of the short residence time.

Direct application of the Bray criterion for sudden freezing does not yield the best results; however, an equilibrium margin applied to the basic curve increases the performance. Further study in this area should indicate an optimum equilibrium margin.

Hydrogen may not be the ideal species to indicate the freeze point in determining the optimum nozzle profile for this system. Other possibilities, including combinations of species, should be investigated.

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TABLE II

FREEZE POINT LOCATION

Area Ratio	$\frac{B}{d\ /dL}$	Area Ratio	$\frac{B}{d\ /dL}$
1.083	.0036307	1.903	.039031
1.124	.0045955	2.079	.052248
1.168	.0056646	2.251	.067470
1.213	.0068524	2.420	.084753
1.259	.0081592	3.976	.365240
1.353	.0111240	5.902	1.102000
1.539	.0184950	7.891	2.687200
1.723	.0277860	13.355	39.807000

TABLE III

MAXIMUM EXPANSION ANGLE

	Half-angle (Degrees)			
Area Ratio	Run 1-C	Run 1-CM	Run 2-C	Run 3-CM
1.04	87.69	86.54	85.20	44.76
1.15	86.00	84.01	81.70	29.75
1.40	79.73	74.79	69.31	12.44
1.77	64.03	53.86	44.59	4.70
1.92	56.21	44.89	33.65	3.42
2.14	44.75	33.46	25.45	2.27
2.21	41.35	30.40	22.90	2.02
2.35	35.12	25.12	18.66	1.61
2.50	29.38	20.58	15.13	1.29
2.80	20.68	14.13	10.27	0.87
3.20	13.39	9.02	6.52	0.55
4.00	6.40	4.28	3.08	0.26
5.00	3.07	2.05	1.47	0.12

TABLE IV

NOZZLE PARAMETERS

Run	Throat Radius (ft)	Throat Area (ft^2)	
1-S	0.167	0.0873	Circular arc to 15° straight expansion.
1-C	0.167	0.0873	Circular arc to 45° ; then 45° straight to 45° allowable contour; then contoured with EM = 1.0 to point of coincidence with Run 1-S; then 15° straight expansion.
1-CM	0.167	0.0873	Same as Run 1-C except contour is with EM = 1.5.
2-S	0.08	0.0201	Same as Run 1-S except different size throat.
2-C	0.08	0.0201	Same as Run 1-C except different size throat.
3-S	0.01	0.003142	Same as Run 1-S except different size throat.
3-CM	0.01	0.003142	Circular arc to 30° ; then 30° straight to 30° allowable contour; then contoured with EM = 1.5 to area ratio of 4.0; then 15° straight expansion.

TABLE V

NOZZLE GEOMETRY FOR RUN 1-S

Length (ft)	Radius (ft)	Area (ft^2)	Area Ratio
0.000	0.167	0.0873	1.000
0.204	0.219	0.1504	1.723
0.230	0.226	0.1601	1.834
0.282	0.240	0.1805	2.068
0.330	0.253	0.2005	2.297
0.399	0.271	0.2308	2.654
0.461	0.288	0.2600	2.979
0.506	0.300	0.2825	3.237
0.577	0.319	0.3196	3.662
0.629	0.333	0.3484	3.992
0.697	0.351	0.3879	4.444
0.817	0.384	0.4631	5.306
1.103	0.461	0.668	7.762
1.294	0.513	0.8254	9.458
1.747	0.634	1.2634	14.476
2.160	0.745	1.7438	19.982
2.553	0.851	2.2734	26.050
3.261	1.042	3.4081	39.052

TABLE VI

NOZZLE GEOMETRY FOR RUN 1-C

Length (ft)	Radius (ft)	Area (ft^2)	Area Ratio
0.000	0.167	0.0873	1.000
0.081	0.219	0.1504	1.723
0.101	0.234	0.1715	1.965
0.110	0.249	0.1950	2.234
0.139	0.267	0.2234	2.560
0.187	0.283	0.2514	2.881
0.272	0.301	0.2839	3.253
0.328	0.309	0.3003	3.441
0.428	0.322	0.3251	3.726
0.553	0.334	0.3511	4.023
0.685	0.354	0.3943	4.518
0.840	0.395	0.4896	5.610
1.002	0.439	0.6052	6.934
1.199	0.492	0.7606	8.715
1.563	0.589	1.0907	12.497
2.276	0.780	1.9132	21.923
2.727	0.901	2.5514	29.235
3.692	1.160	4.2247	48.410

TABLE VII

NOZZLE GEOMETRY FOR RUN 1-CM

Length (ft)	Radius (ft)	Area (ft^2)	Area Ratio
0.000	0.167	0.0873	1.000
0.080	0.219	0.1507	1.727
0.093	0.232	0.1694	1.941
0.102	0.240	0.1804	2.106
0.115	0.248	0.1936	2.210
0.137	0.259	0.2108	2.414
0.182	0.274	0.2366	2.711
0.312	0.301	0.2838	3.251
0.449	0.318	0.3169	3.631
0.640	0.336	0.3539	4.055
0.701	0.352	0.3897	4.466
0.837	0.388	0.4740	5.431
0.961	0.423	0.5609	6.427
1.263	0.505	0.8005	9.173
1.836	0.658	1.3610	15.594
2.699	0.890	2.4886	28.516
3.591	1.131	4.0184	46.046

TABLE VIII

NOZZLE GEOMETRY FOR RUN 2-S

Length (ft)	Radius (ft)	Area (ft^2)	Area Ratio
0.000	0.080	0.0201	1.000
0.023	0.085	0.0226	1.124
0.035	0.088	0.0245	1.217
0.069	0.097	0.0298	1.481
0.103	0.107	0.0356	1.772
0.149	0.119	0.0442	2.198
0.170	0.124	0.0486	2.417
0.198	0.132	0.0546	2.717
0.246	0.145	0.0658	3.270
0.275	0.153	0.0731	3.636
0.312	0.163	0.0826	4.125
0.349	0.172	0.0932	4.635
0.422	0.192	0.1155	5.746
0.505	0.214	0.1440	7.160
0.673	0.259	0.2108	10.482
0.916	0.324	0.3303	16.422
1.255	0.415	0.5412	26.911
1.463	0.471	0.6963	34.625
1.631	0.516	0.8356	41.552

TABLE IX

NOZZLE GEOMETRY FOR RUN 2-C

Length (ft)	Radius (ft)	Area (ft^2)	Area Ratio
0.000	0.080	0.0201	1.000
0.017	0.085	0.0226	1.123
0.024	0.091	0.0260	1.295
0.030	0.097	0.0296	1.473
0.038	0.105	0.0346	1.722
0.051	0.114	0.0414	2.046
0.067	0.122	0.0465	2.314
0.095	0.130	0.0527	2.621
0.156	0.140	0.0616	3.062
0.234	0.149	0.0693	3.445
0.308	0.161	0.0819	4.073
0.356	0.175	0.0958	4.764
0.442	0.198	0.1225	6.093
0.624	0.246	0.1895	9.425
0.801	0.293	0.2700	13.424
0.981	0.342	0.3667	18.236
1.320	0.432	0.5875	29.216
1.528	0.488	0.7486	37.160
1.669	0.526	0.8689	43.092

TABLE X

NOZZLE GEOMETRY FOR RUN 3-S

Length x 10^2 (ft)	Radius x 10^2 (ft)	Area x 10^3 (ft^2)	Area Ratio
0.000	1.000	0.3142	1.000
0.204	1.041	0.3402	1.083
0.432	1.101	0.3810	1.212
0.808	1.202	0.4538	1.444
1.607	1.417	0.6308	2.008
2.368	1.620	0.8246	2.625
2.992	1.787	1.0035	3.194
3.935	2.040	1.3079	4.163
5.991	2.591	2.1093	6.714
9.933	3.647	4.1794	13.303
14.211	4.794	7.2194	22.980
18.490	5.940	11.0843	35.282

TABLE XI

NOZZLE GEOMETRY FOR RUN 3-CM

Length x 10^2 (ft)	Radius x 10^2 (ft)	Area x 10^3 (ft^2)	Area Ratio
0.000	1.000	0.3142	1.000
0.176	1.041	0.3402	1.090
0.371	1.132	0.4023	1.281
0.563	1.183	0.4400	1.401
1.772	1.334	0.5593	1.780
3.199	1.423	0.6358	2.024
6.940	1.553	0.7576	2.412
12.555	1.668	0.8738	2.781
29.700	1.810	1.0289	3.275
39.992	1.917	1.1547	3.676
52.417	2.006	1.2639	4.023
57.021	2.147	1.4488	4.612
57.671	2.325	1.6981	5.406
59.936	2.985	2.7995	8.911
63.627	3.961	4.9299	15.692
66.395	4.705	6.9552	22.139
68.324	5.222	8.5669	27.270
70.170	5.717	10.2664	32.679
72.015	6.211	12.1190	38.576
72.938	6.458	13.1030	41.708

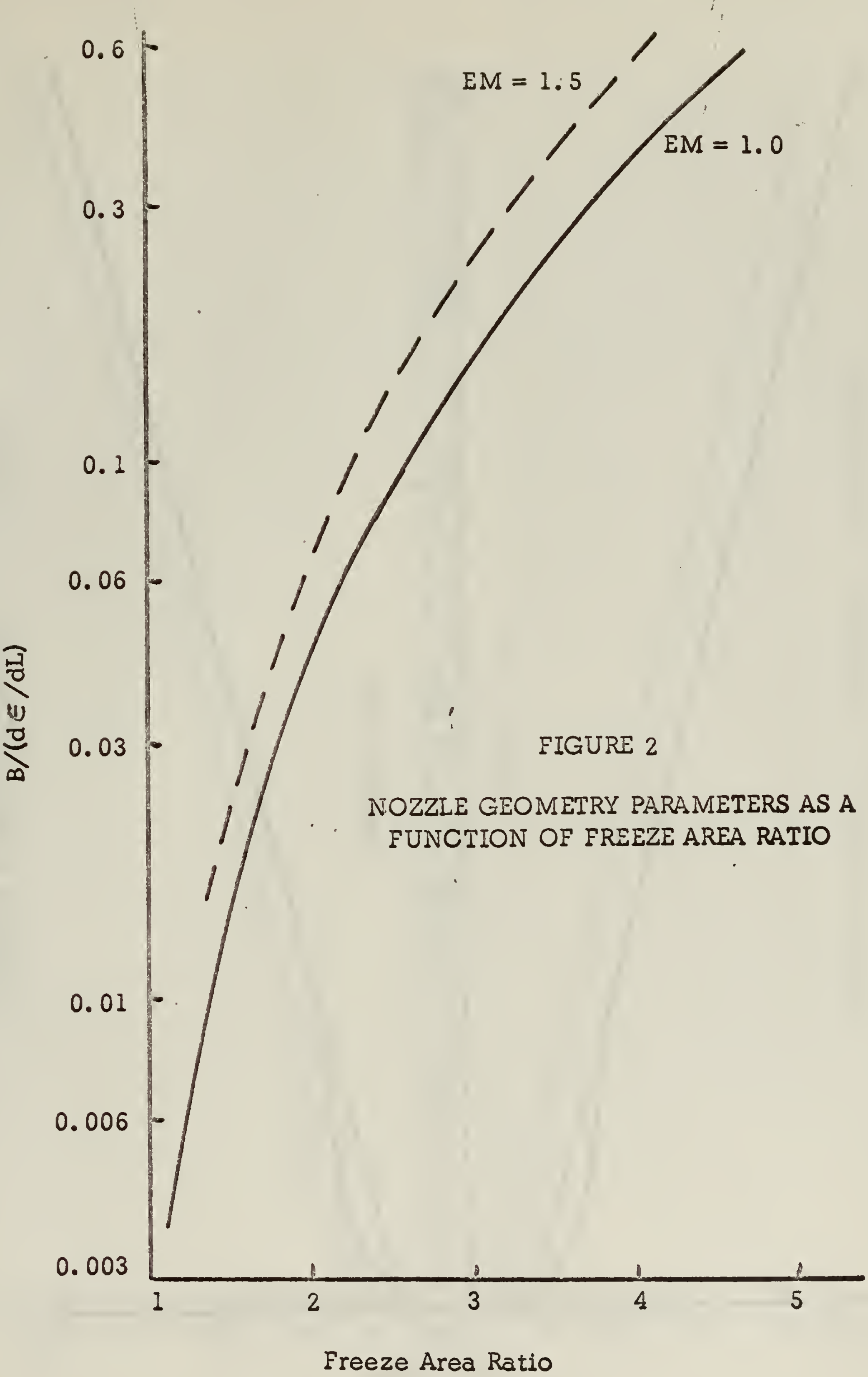


FIGURE 2

NOZZLE GEOMETRY PARAMETERS AS A FUNCTION OF FREEZE AREA RATIO

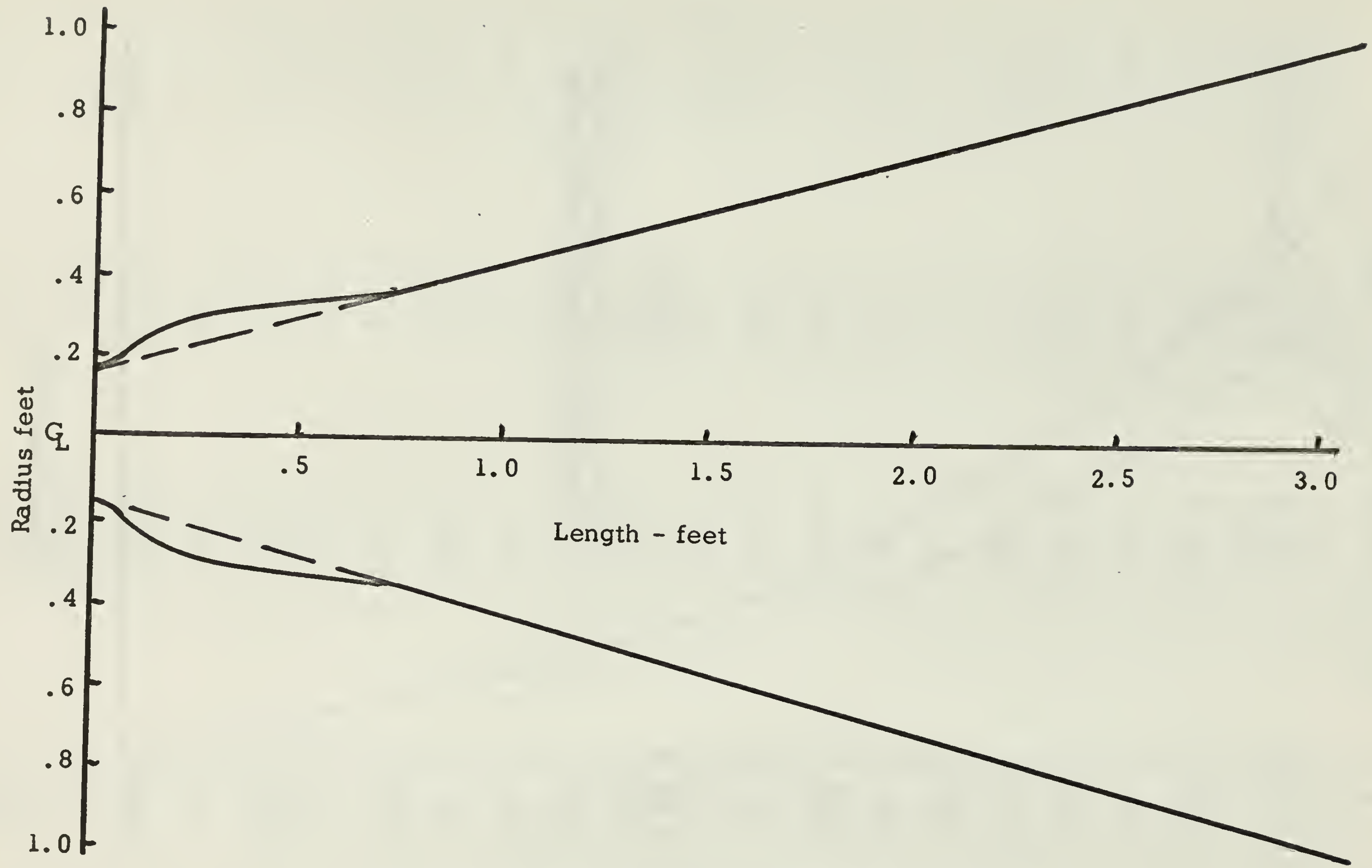


FIGURE 3 NOZZLE GEOMERY, r^* = 2 INCHES

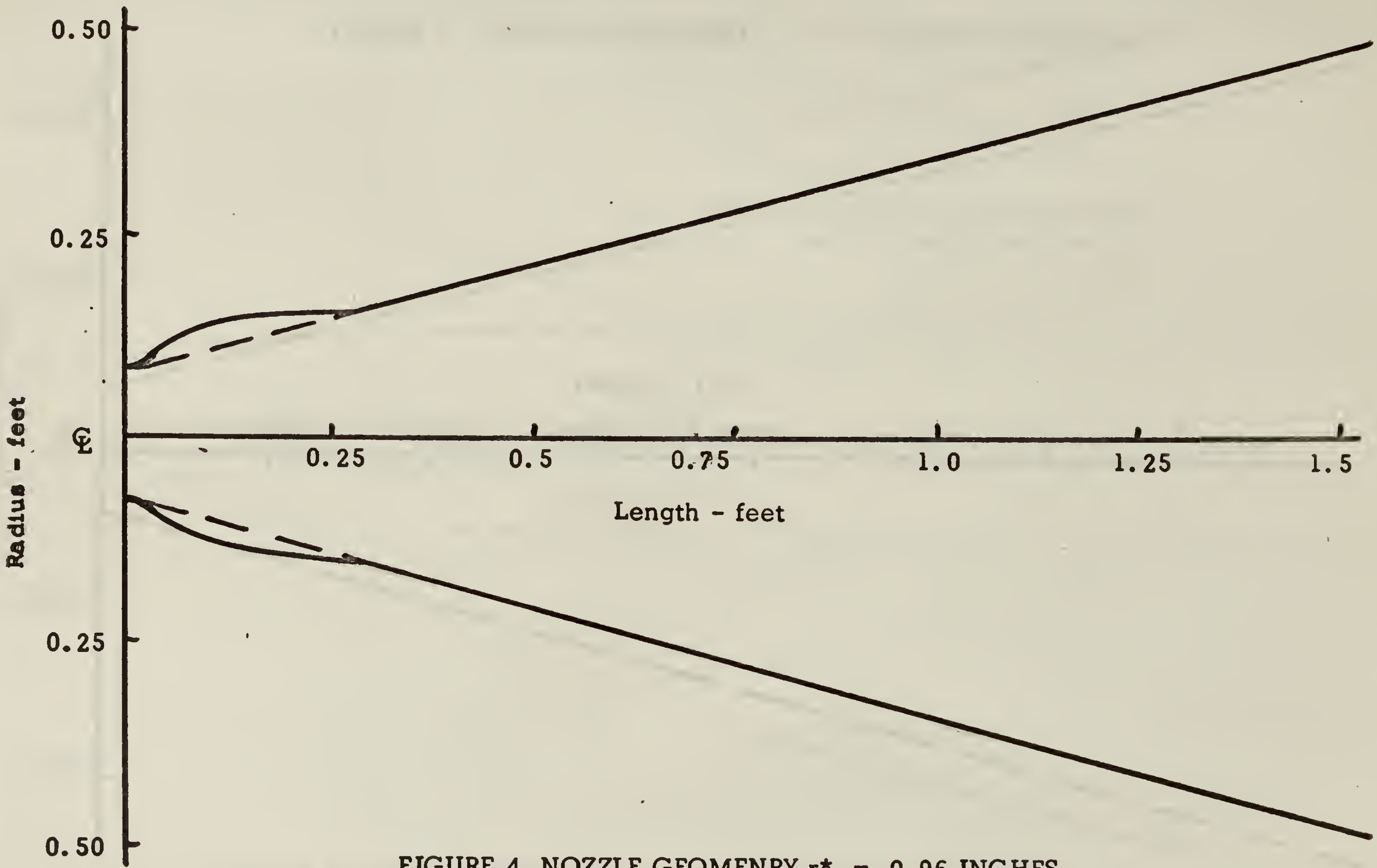


FIGURE 4 NOZZLE GEOMENRY, r^* = 0.96 INCHES

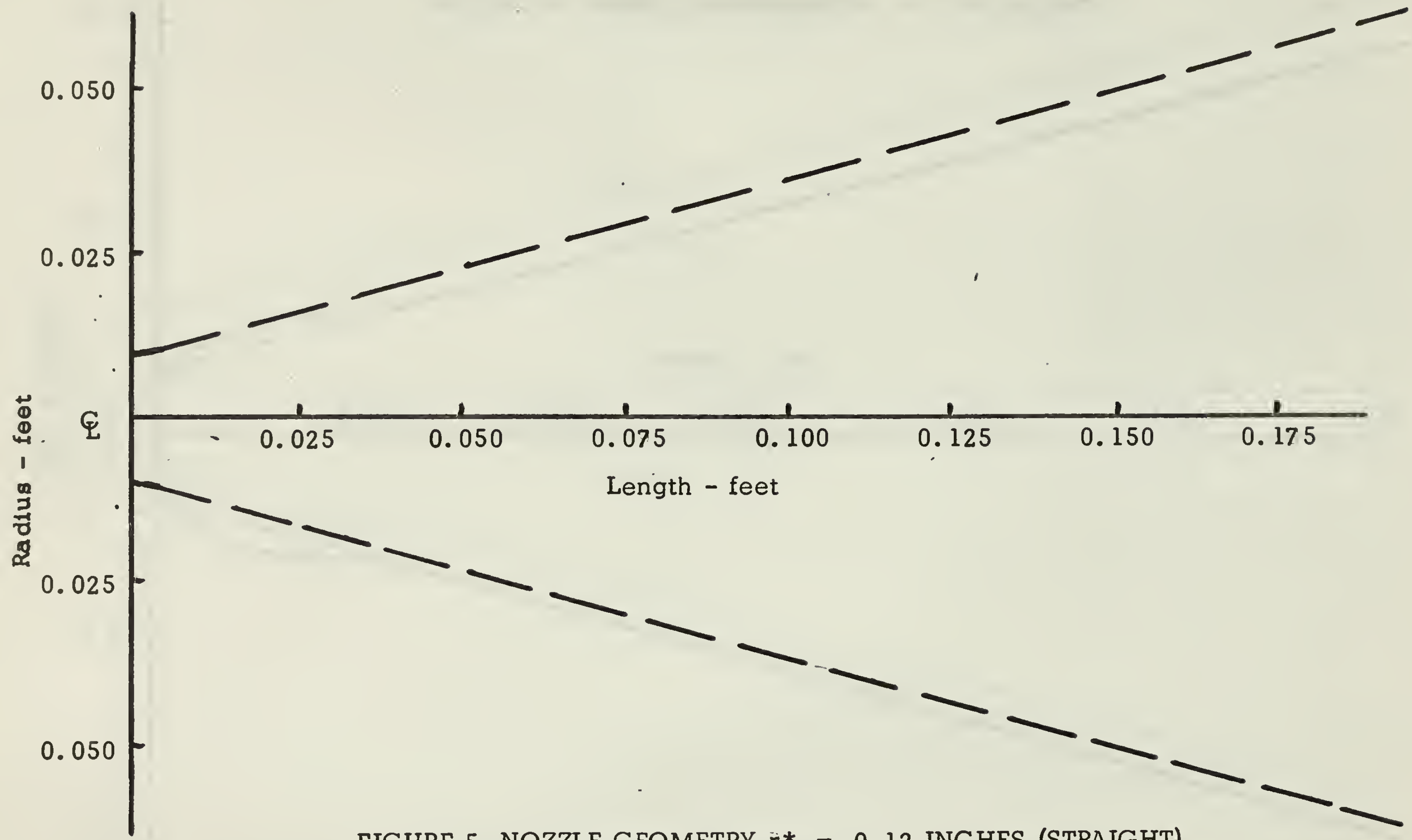


FIGURE 5 NOZZLE GEOMETRY, r^* = 0.12 INCHES (STRAIGHT)

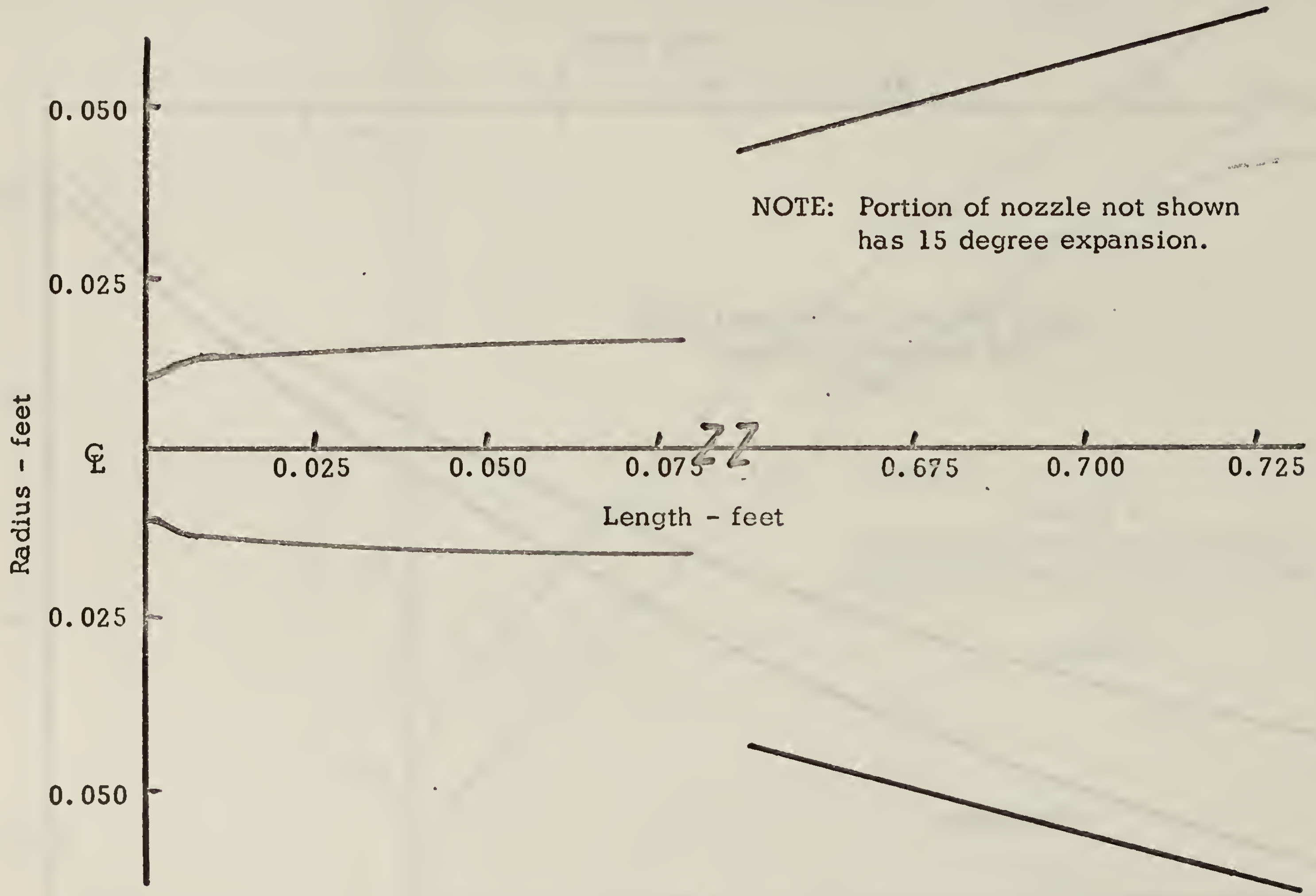


FIGURE 6 NOZZLE GEOMETRY, r^* = 0.12 INCHES (CONTOURED)

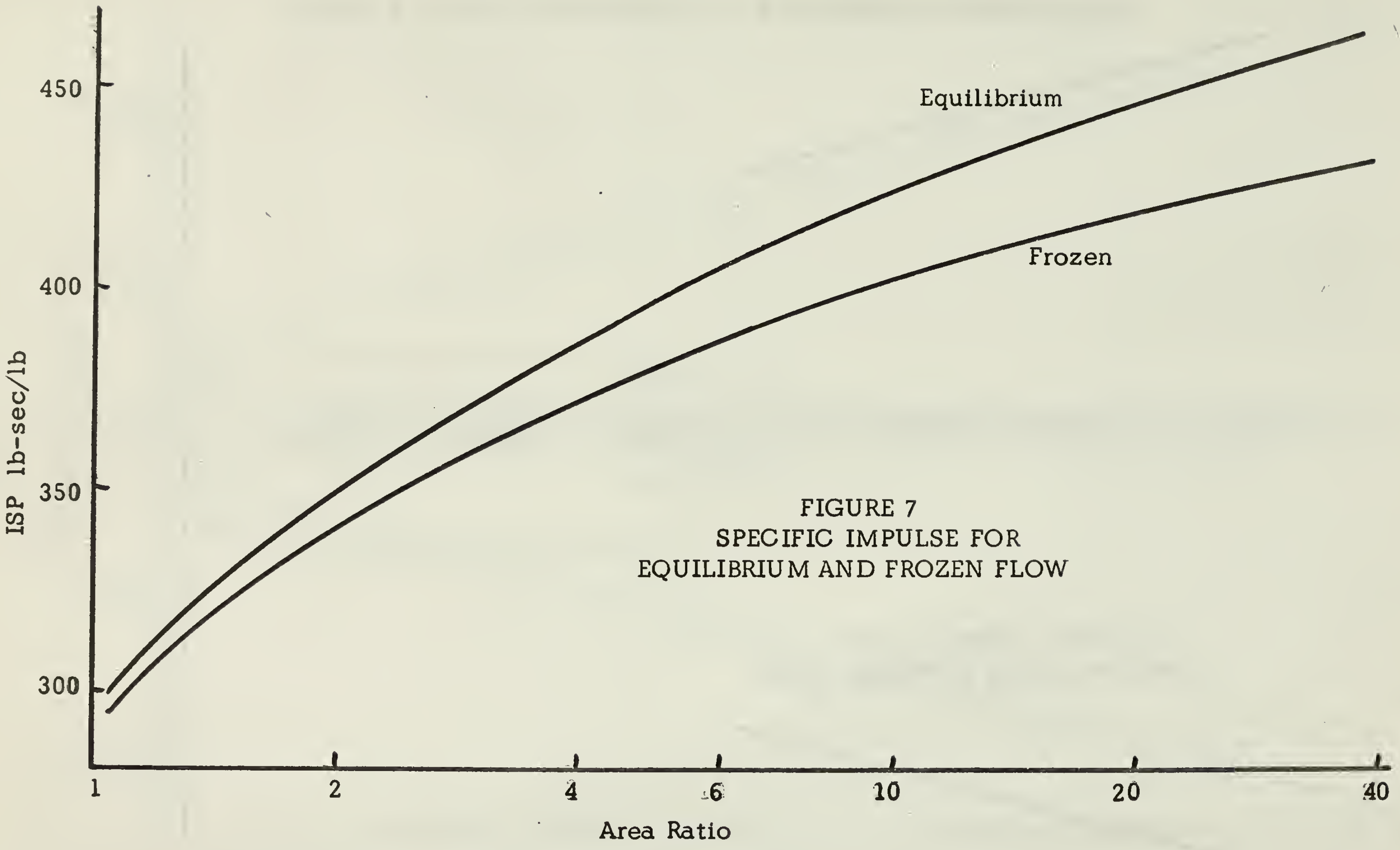


FIGURE 7
SPECIFIC IMPULSE FOR
EQUILIBRIUM AND FROZEN FLOW

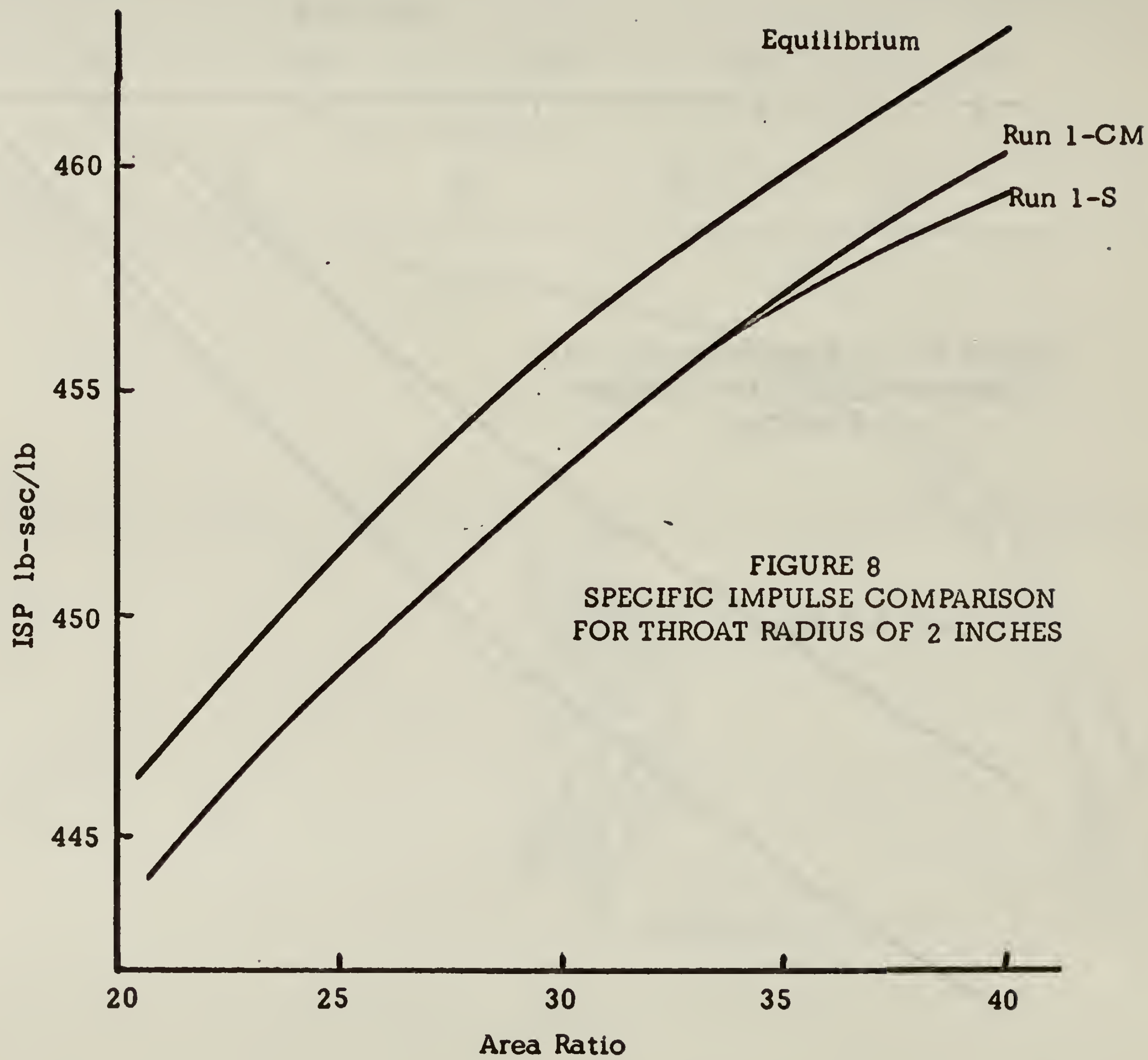


FIGURE 8
SPECIFIC IMPULSE COMPARISON
FOR THROAT RADIUS OF 2 INCHES

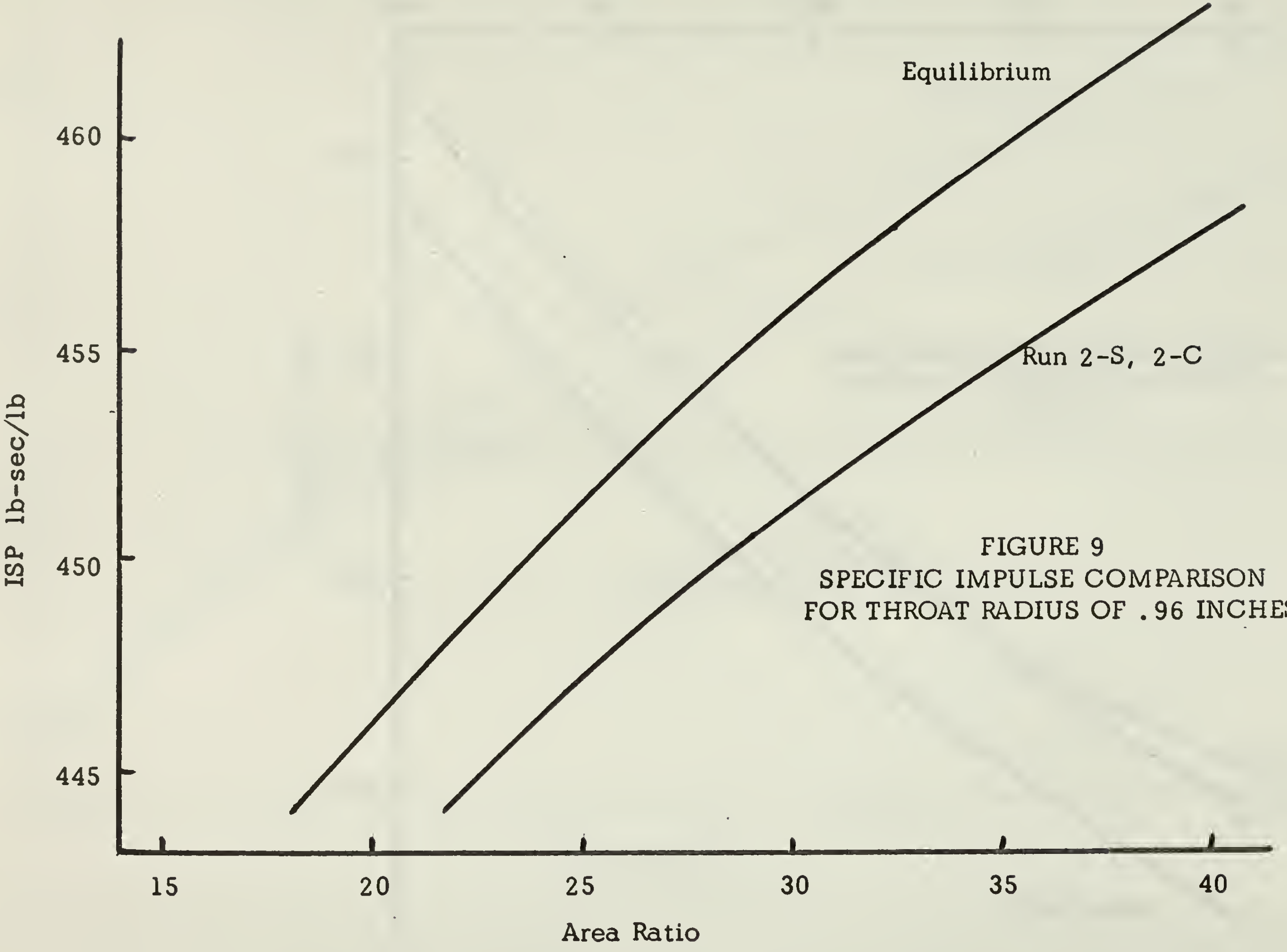
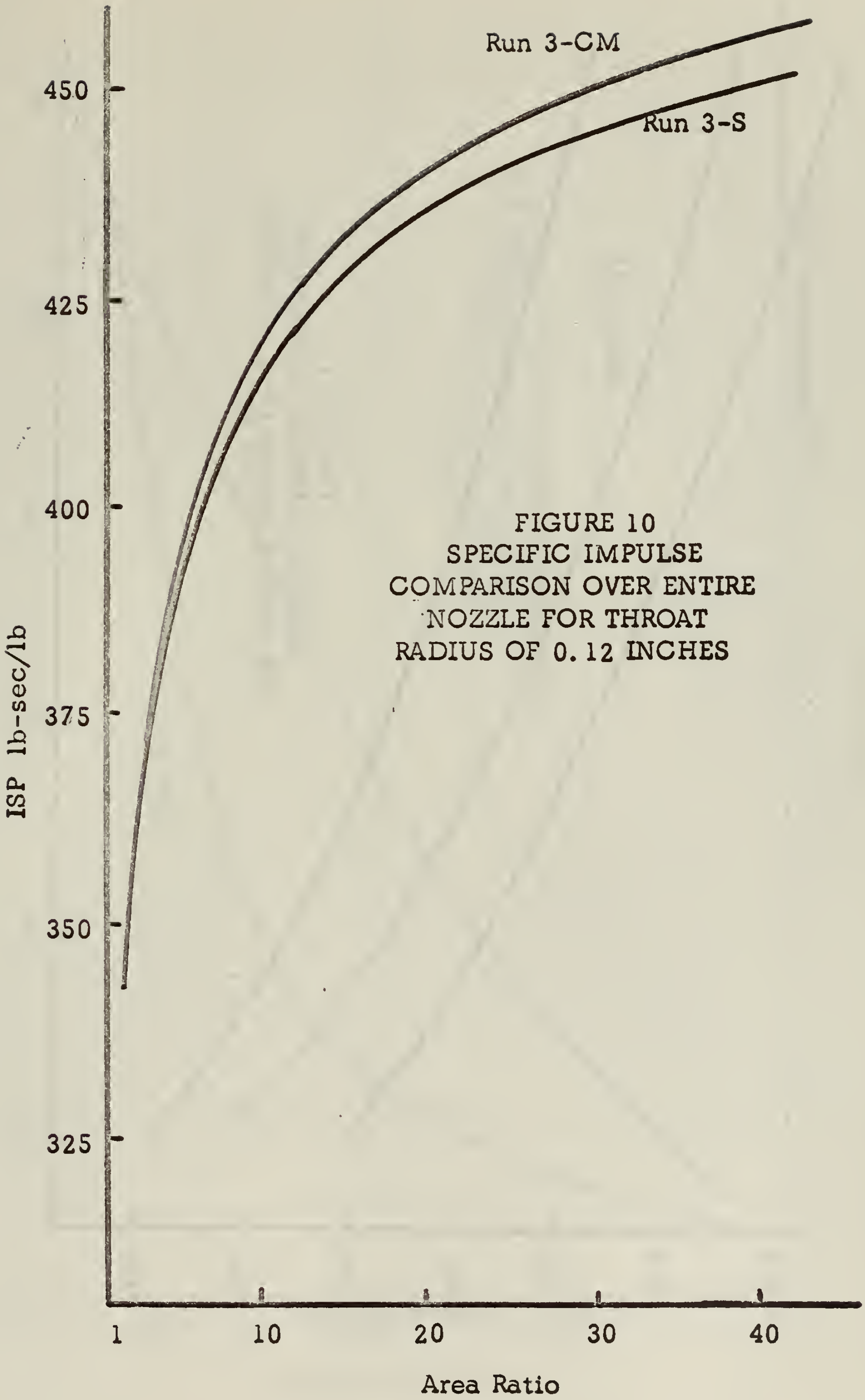


FIGURE 9
SPECIFIC IMPULSE COMPARISON
FOR THROAT RADIUS OF .96 INCHES


Run 3-CM
Run 3-S
FIGURE 10
SPECIFIC IMPULSE
COMPARISON OVER ENTIRE
NOZZLE FOR THROAT
RADIUS OF 0.12 INCHES
ISP lb-sec/lb
450
425
400
375
350
325
1
10
20
30
40
Area Ratio

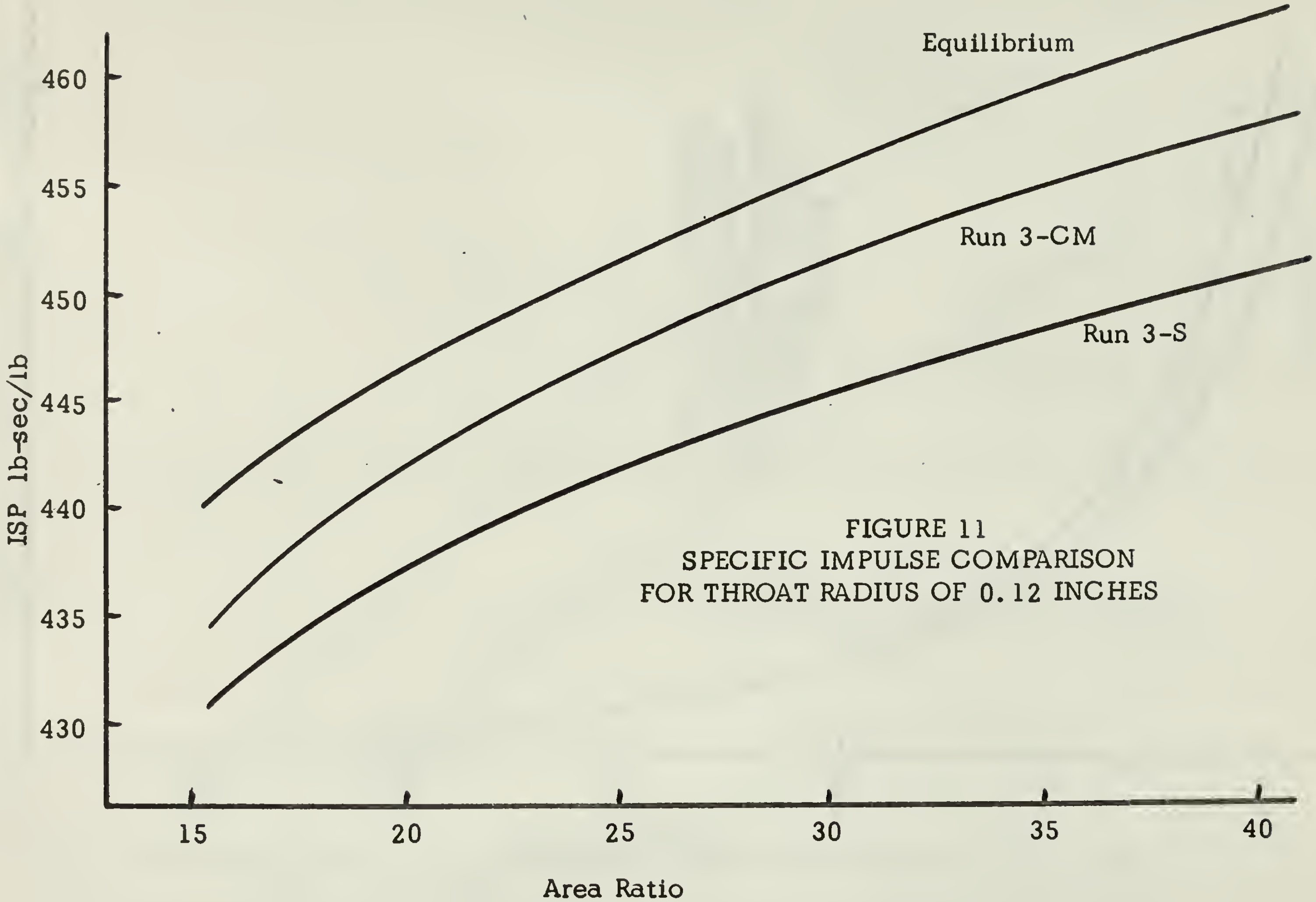


FIGURE 11
SPECIFIC IMPULSE COMPARISON
FOR THROAT RADIUS OF 0.12 INCHES

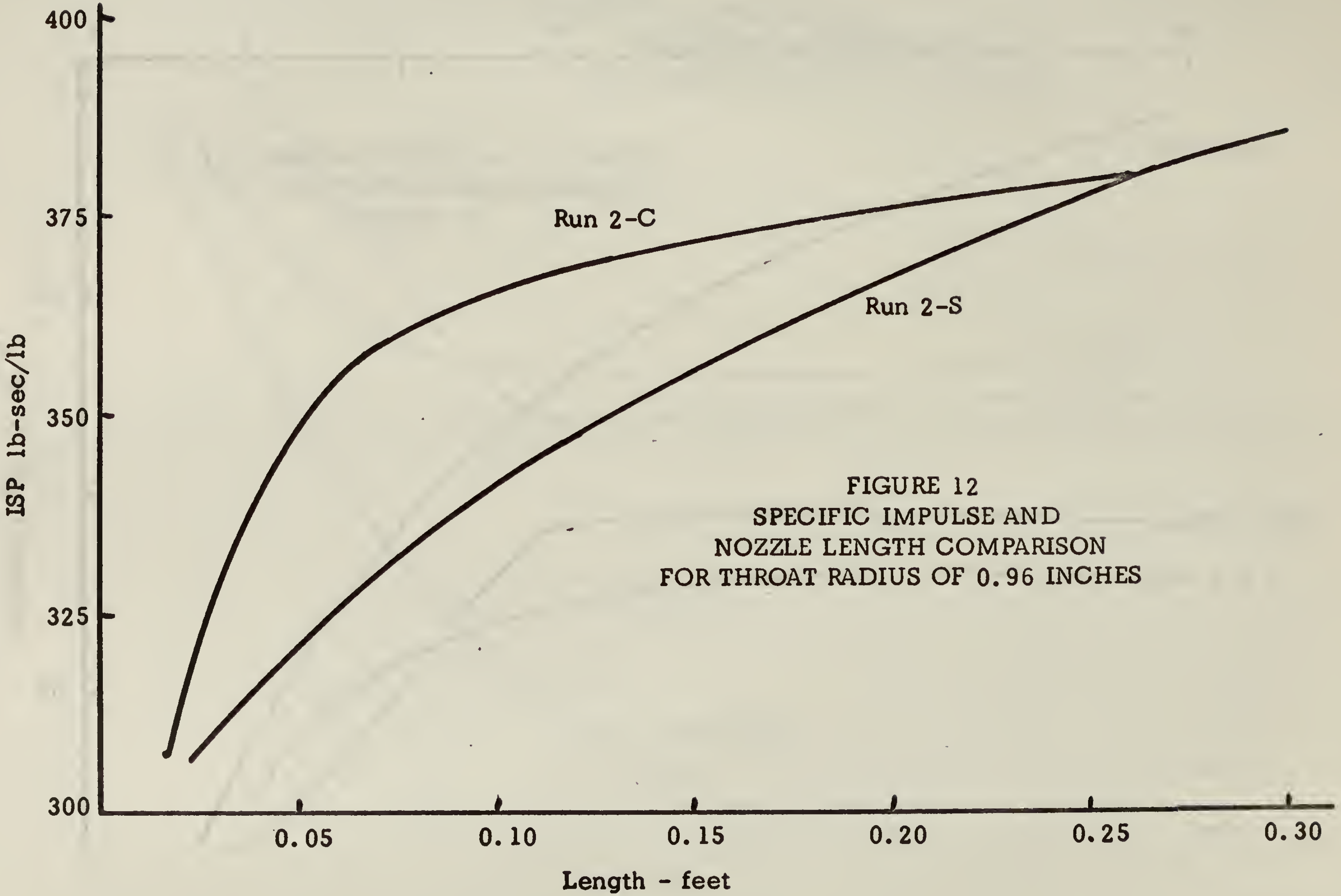


FIGURE 12
SPECIFIC IMPULSE AND
NOZZLE LENGTH COMPARISON
FOR THROAT RADIUS OF 0.96 INCHES

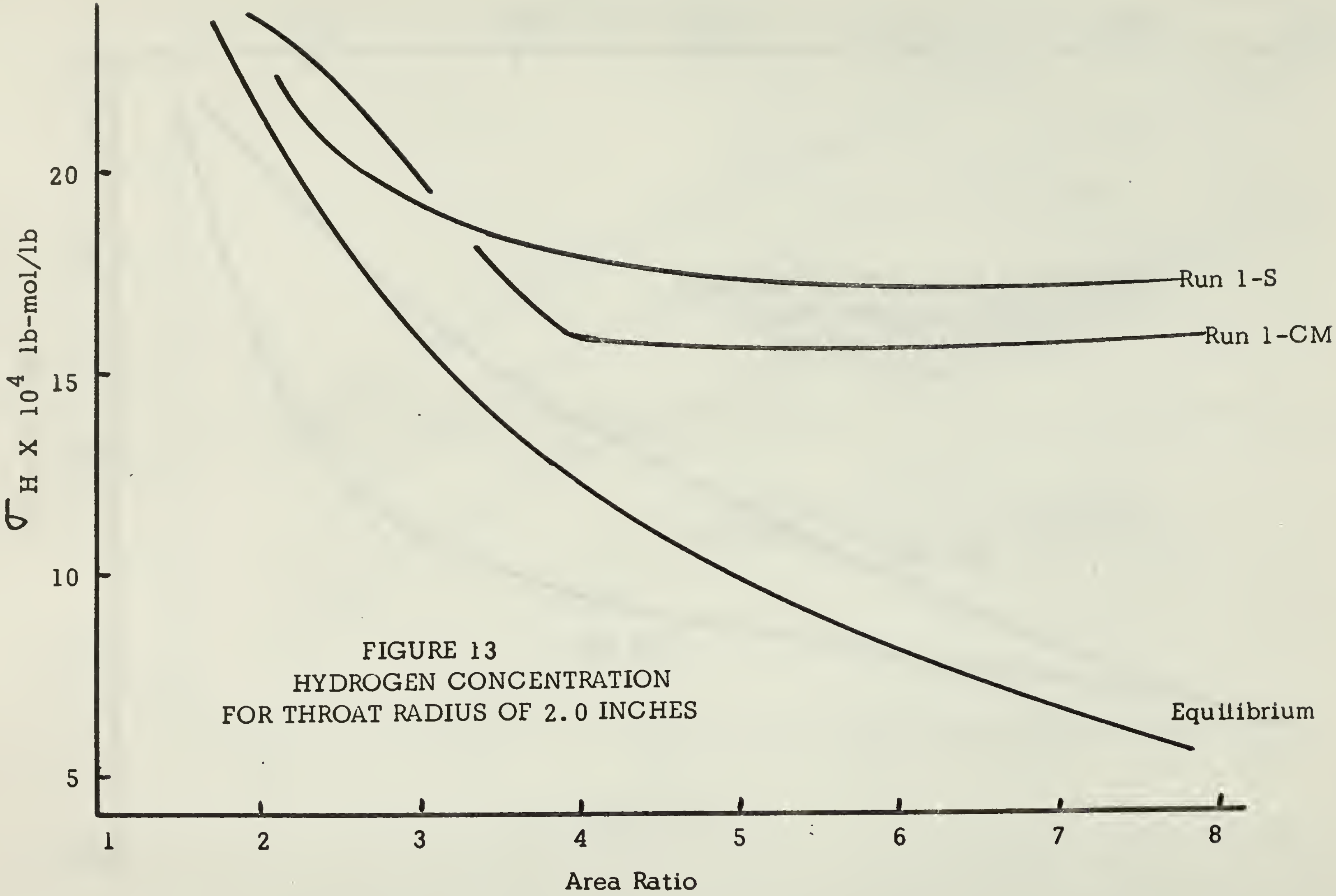
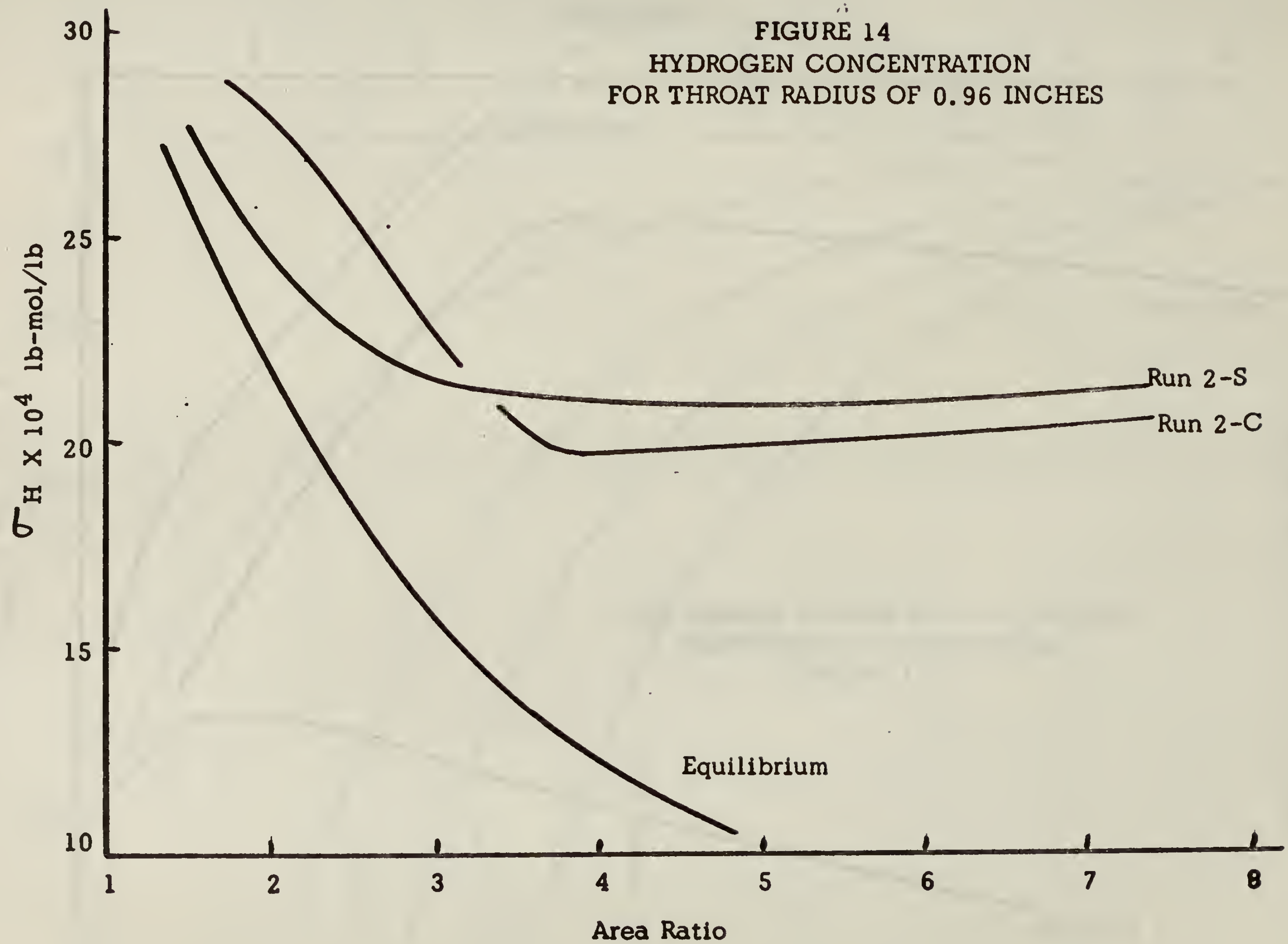


FIGURE 13
HYDROGEN CONCENTRATION
FOR THROAT RADIUS OF 2.0 INCHES

FIGURE 14
HYDROGEN CONCENTRATION
FOR THROAT RADIUS OF 0.96 INCHES



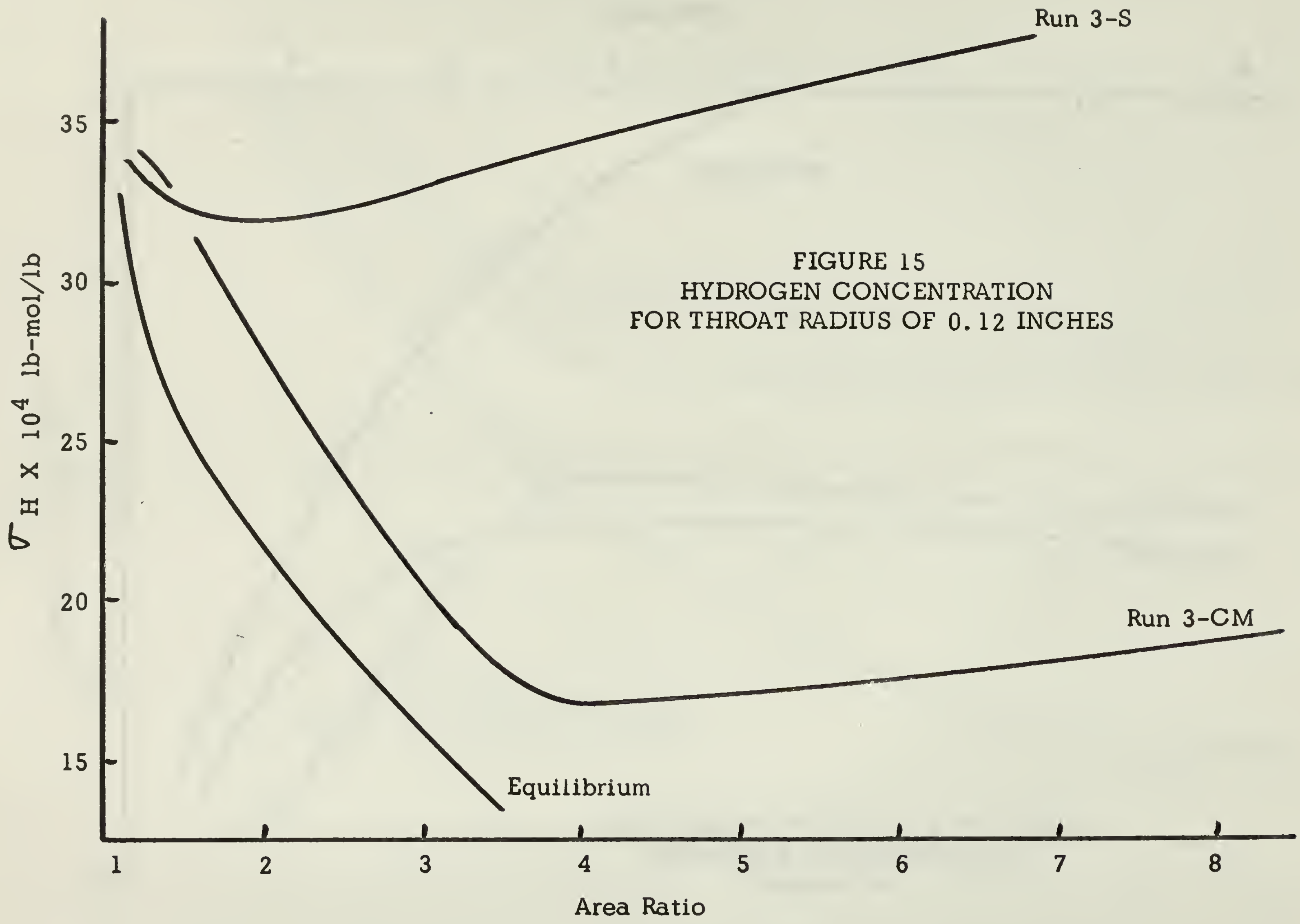


FIGURE 15
HYDROGEN CONCENTRATION
FOR THROAT RADIUS OF 0.12 INCHES

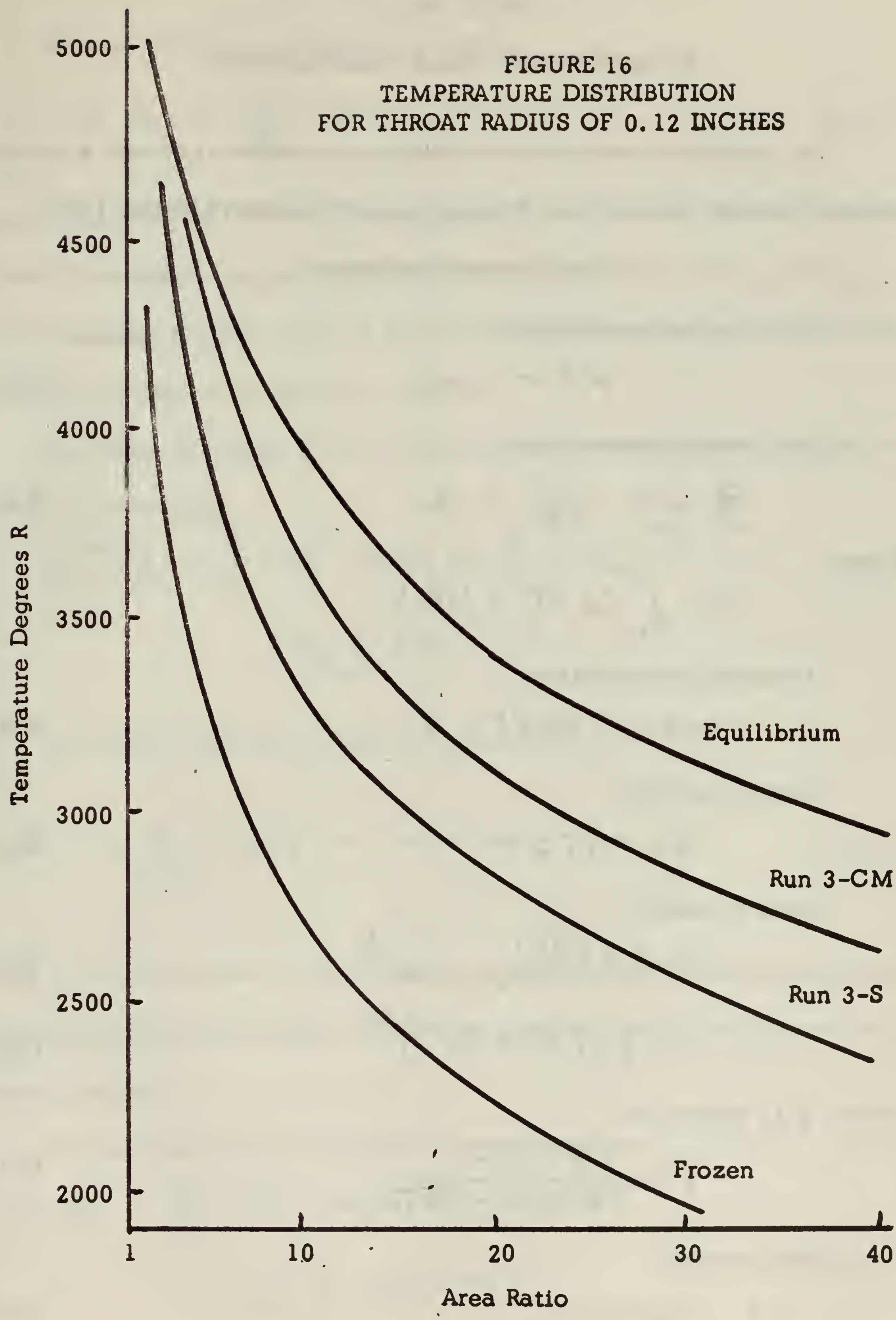


FIGURE 16
TEMPERATURE DISTRIBUTION
FOR THROAT RADIUS OF 0.12 INCHES
5000
4500
4000
3500
3000
2500
2000
Temperature Degrees R
Equilibrium
Run 3-CM
Run 3-S
Frozen
1
10
20
30
40
Area Ratio

APPENDIX I

EQUATIONS FOR EXACT CALCULATIONS

The equations involved in the analysis of nozzle flow with a chemical reaction include those of gas dynamics and of reaction kinetics [18].

Gas Dynamic Equations

Overall mass conservation:

$$\rho A v = \dot{m} \tag{I-1}$$

Total energy conservation:

$$\sum_{i=1}^{n} h_i \sigma_i + \frac{v^2}{2gJ} = H_o \tag{I-2}$$

where:

$$h_i = \int_{T_b}^{T} C_{P_i}\, dT + (H_{fi})_b$$

Momentum conservation:

$$v\, dv + g/\rho\, dP = 0 \tag{I-3}$$

Equation of state:

$$P = \rho R T \Sigma \sigma \tag{I-4}$$

Speed of sound:

$$C = \left[g \left(\frac{\partial P}{\partial \rho} \right)_{S, \sigma_1, \ldots \sigma_n} \right]^{1/2} \tag{I-5}$$

$$= \left[g \gamma R T \Sigma \sigma_i \right]^{1/2} \tag{I-6}$$

where γ is defined as:

$$\gamma = \frac{J \Sigma C_{P_i} \sigma_i}{J \Sigma C_{P_i} \sigma_i - R \Sigma \sigma_i} \tag{I-7}$$

Mach number:

$$M = \frac{V}{C} \tag{I-8}$$

Reaction Kinetics Equations

General form of n_r chemical reactions:

$$\sum \nu'_{ij} M_i \underset{k_{bj}}{\overset{k_{fj}}{\rightleftharpoons}} \sum \nu''_{ij} M_i \tag{I-9}$$

where ν'_{ij} and ν''_{ij} are the stoichiometric coefficients of the i^{th} species in the j^{th} reaction, reactants and products respectively, and k_{fj} and k_{bj} are the specific reaction rates of the forward and backward chemical changes in the j^{th} reaction of the chemical system.

The rates of change of the concentration of the species M_i are determined by the relation:

$$\left.\frac{\partial [M_i]}{\partial t}\right)_\rho = \sum_{j=1}^{n_r} (\nu''_{ij} - \nu'_{ij}) \left\{ k_{fj} \prod_{k=1}^{n} [M_k]^{\nu'_{kj}} - k_{bj} \prod_{k=1}^{n} [M_k]^{\nu''_{kj}} \right\} \tag{I-10}$$

The atomic species continuity equations are:

$$\sigma_i + \sum_{j=n_a+1}^{n} B_{ij}\sigma_j = \text{constant} \qquad (i = 1, 2, \cdots, n_a) \tag{I-11}$$

where B_{ij} is the number of the i^{th} atomic species in the j^{th} molecular species, n designates the total number of chemical species, and n_a is the number of atomic species.

The molecular species continuity equations are:

$$\rho v \sigma'_i = \sum_{j=1}^{n_r} (\nu''_{ij} - \nu'_{ij}) \left[k_{fj} \prod_{k=1}^{n} (\rho\sigma_k)^{\nu'_{kj}} - k_{bj} \prod_{k=1}^{n} (\rho\sigma_k)^{\nu''_{kj}} \right]_{i = n_a+1, n_a+2, \ldots n} \tag{I-12}$$

It should be noted that of the n equations represented by (I-11) and (I-12), only n-1 are independent because of the overall mass conservation equation (I-1). The exact calculations involve the simultaneous solution of equations (I-1), (I-2), (I-3), (I-4), (I-10), (I-11), and (I-12).

APPENDIX II

EQUILIBRIUM AND FROZEN RESULTS

TABLE II-1

Equilibrium Composition Values

Area Ratio	Pressure (Atmos)	Pressure Ratio (P_C/P)	Temp Deg K	Gamma	Specific Heat Cal/gm-°K	Enthalpy Cal/gm
Chamber	20.414	1.000	3439	1.1313	2.9563	0
Throat	11.811	1.728	3274	1.1294	2.7698	-277.8
1.083	8.165	2.500	3166	1.1288	2.6193	-455.7
1.124	7.423	2.750	3139	1.1288	2.5773	-500.4
1.168	6.805	3.000	3114	1.1288	2.5380	-540.8
1.213	6.281	3.250	3091	1.1288	2.5010	-577.6
1.259	5.832	3.500	3070	1.1289	2.4660	-611.3
1.353	5.103	4.000	3033	1.1291	2.4013	-671.5
1.539	4.083	5.000	2971	1.1297	2.2887	-770.0
1.723	3.402	6.000	2920	1.1304	2.1932	-848.8
1.903	2.916	7.000	2877	1.1313	2.1105	-913.8
2.079	2.552	8.000	2840	1.1322	2.0376	-969.3
2.251	2.268	9.000	2807	1.1332	1.9727	-1017.6
2.420	2.041	10.000	2778	1.1342	1.9144	-1060.2
3.976	1.021	20.000	2582	1.1442	1.5364	-1327.5
5.902	0.600	34.020	2425	1.1567	1.2786	-1517.3
7.891	0.408	50.000	2306	1.1682	1.1237	-1646.5
13.355	0.204	100.000	2083	1.1913	0.9259	-1861.6
45.521	0.041	500.000	1573	1.2311	0.7515	-2275.2
77.299	0.020	5000.000	989	1.2437	0.7190	-2419.0

TABLE II-2

Equilibrium Composition Values

Area Ratio	Mean Mol. wt.	Mach Number	C* Ft/sec	C_F	Specific Impulse (lb-sec/lb) $I_{sp})_v$	I_{sp}
Chamber	13.043	0.000	----	----	----	----
Throat	13.223	1.000	7655	.654	293.1	155.5
1.083	13.341	1.308	7655	.837	302.2	199.1
1.124	13.370	1.379	7655	.877	305.9	208.7
1.168	13.397	1.440	7655	.912	309.6	216.9
1.213	13.421	1.495	7655	.942	313.0	224.2
1.259	13.444	1.545	7655	.969	316.3	230.6
1.353	13.484	1.631	7655	1.016	322.2	241.7
1.539	13.548	1.769	7655	1.088	332.1	258.8
1.723	13.599	1.876	7655	1.142	340.0	271.7
1.903	13.641	1.963	7655	1.185	346.6	282.0
2.079	13.677	2.037	7655	1.221	352.2	290.4
2.251	13.707	2.101	7655	1.251	357.1	297.6
2.420	13.733	2.157	7655	1.277	361.3	303.7
3.976	13.887	2.506	7655	1.429	387.2	339.9
5.902	13.978	2.759	7655	1.527	404.6	363.3
7.891	14.028	2.938	7655	1.591	416.1	378.5
13.355	14.082	3.261	7655	1.692	434.2	402.5
45.521	14.111	4.085	7655	1.870	466.6	444.9
77.299	14.112	4.479	7655	1.928	477.2	458.8

TABLE II-3

Frozen Composition Values

Area Ratio	Pressure (Atmos)	Pressure Ratio (P_o/P)	Temp Deg K	Gamma	Specific Heat Cal/gm-°K	Enthalpy Cal/gm
Chamber	20.414	1.000	3439	1.2057	.8932	0
Throat	11.483	1.778	3115	1.2096	.8792	-287.1
1.065	8.165	2.500	2936	1.2123	.8702	-444.2
1.101	7.423	2.750	2887	1.2130	.8676	-486.5
1.139	6.805	3.000	2843	1.2137	.8652	-524.5
1.179	6.281	3.250	2803	1.2144	.8629	-558.9
1.219	5.832	3.500	2767	1.2151	.8608	-590.4
1.301	5.103	4.000	2702	1.2162	.8570	-646.0
1.464	4.083	5.000	2597	1.2183	.8503	-736.1
1.624	3.402	6.000	2513	1.2201	.8447	-807.0
1.779	2.916	7.000	2444	1.2216	.8398	-865.2
1.931	2.552	8.000	2385	1.2230	.8355	-914.3
2.078	2.268	9.000	2334	1.2243	.8316	-956.7
2.222	2.041	10.000	2290	1.2255	.8281	-993.8
3.523	1.021	20.000	2012	1.2339	.8037	-1220.7
5.098	.600	34.023	1817	1.2413	.7837	-1375.5
6.702	.408	50.000	1684	1.2472	.7686	-1478.2
11.048	.204	100.000	1464	1.2590	.7406	-1644.2
35.866	.041	500.00	1035	1.2924	.6735	-1948.5
59.600	.020	1000.000	882	1.3074	.6480	-2049.5

TABLE II-4

Frozen Composition Values

Area Ratio	Mean Mol. wt.	Mach Number	C* Ft/sec	C_F	Specific Impulse (lb-sec/lb) $I_{sp})v$	I_{sp}
Chamber	13.043	0	----	----	----	----
Throat	13.043	1.000	7473	.680	288.7	158.0
1.065	13.043	1.280	7473	.846	295.6	196.6
1.101	13.043	1.350	7473	.886	298.8	205.7
1.139	13.043	1.412	7473	.920	301.8	213.6
1.179	13.043	1.468	7473	.949	304.8	220.5
1.219	13.043	1.518	7473	.976	307.6	226.6
1.301	13.043	1.606	7473	1.021	312.6	237.1
1.464	13.043	1.748	7473	1.090	321.1	253.1
1.624	13.043	1.859	7473	1.141	327.9	265.0
1.779	13.043	1.950	7473	1.181	333.4	274.4
1.931	13.043	2.028	7473	1.214	338.1	282.1
2.078	13.043	2.096	7473	1.242	342.2	288.5
2.222	13.043	2.156	7473	1.266	345.7	294.1
3.523	13.043	2.541	7473	1.403	366.8	325.9
5.098	13.043	2.830	7473	1.489	380.8	346.0
6.702	13.043	3.039	7473	1.544	389.8	358.6
11.048	13.043	3.422	7473	1.628	403.9	378.2
35.866	13.043	4.373	7473	1.773	428.4	411.8
59.600	13.043	4.830	7473	1.818	436.1	422.3

TABLE II-5

EQUILIBRIUM FLOW SPECIES CONCENTRATIONS

Mol Fractions x10^3

Area Ratio	O_1	H_1	O_2	H_2	OH	H_2O
Chamber	8.16	56.88	7.75	252.15	62.82	612.24
Throat	6.06	49.35	6.14	248.38	52.17	637.90
1.083	4.81	44.33	5.07	246.06	45.20	654.53
1.124	4.51	43.03	4.80	245.50	43.44	658.71
1.168	4.25	41.86	4.56	245.00	41.84	662.49
1.213	4.01	40.77	4.34	244.56	40.38	665.93
1.259	3.80	39.78	4.14	244.16	39.04	669.08
1.353	3.43	37.98	3.79	243.48	36.66	674.67
1.539	2.85	34.99	3.22	242.44	32.76	683.73
1.723	2.43	32.56	2.79	241.69	29.67	690.87
1.903	2.10	30.52	2.44	241.13	27.12	696.69
2.079	1.83	28.76	2.15	240.72	24.98	701.56
2.251	1.61	27.22	1.92	240.40	23.14	705.72
2.420	1.43	25.85	1.72	240.15	21.53	709.32
3.976	0.55	17.19	0.69	239.55	12.16	729.86
5.902	0.21	11.26	0.26	240.17	6.74	741.36
7.891	0.08	7.63	0.11	240.99	3.94	747.24
13.355	0.01	3.04	0.01	242.56	1.12	753.25
45.521	----	0.10	----	243.94	0.01	755.95
77.299	----	0.01	----	243.99	----	755.99

APPENDIX III

EXACT RESULTS

TABLE III-1

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 1-S

Area Ratio	Species Concentration (lb-mol/lb) x 10^4					
	O	H	O_2	H_2	OH	H_2O
1.723	1.79	23.91	2.05	177.83	21.83	507.98
1.834	1.72	23.66	2.02	177.50	21.19	508.75
2.068	1.51	22.45	1.81	176.51	19.27	511.30
2.297	1.33	21.37	1.63	175.72	17.68	513.43
2.645	1.14	20.10	1.41	174.77	15.77	515.96
2.979	1.00	19.21	1.26	174.07	14.35	517.82
3.237	0.92	18.69	1.18	173.63	13.46	518.96
3.662	0.82	18.07	1.06	173.03	12.27	520.48
3.992	0.77	17.73	1.00	172.64	11.53	521.41
4.444	0.71	17.41	0.93	172.18	10.69	522.45
5.306	0.63	17.10	0.84	171.47	9.48	523.91
7.762	0.52	17.15	0.72	170.10	7.48	526.25
9.458	0.47	17.45	0.75	169.33	6.52	527.35
14.476	0.40	18.42	0.61	167.81	4.86	529.23
19.982	0.35	19.29	0.57	166.70	3.77	530.45
26.050	0.31	20.01	0.54	165.84	2.99	531.33
39.052	0.24	21.03	0.51	164.70	1.98	532.47

TABLE III-2

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 1-C

Area Ratio	Species Concentration (lb-mol/lb) x 10^4 O	H	O_2	H_2	OH	H_2O
1.723	1.79	23.91	2.05	177.83	21.80	507.98
1.965	1.71	23.93	2.03	177.06	20.57	509.37
2.234	1.64	24.00	1.99	176.21	19.25	510.84
2.560	1.44	22.90	1.81	175.29	17.41	513.23
2.881	1.22	21.35	1.55	174.46	15.66	515.71
3.253	1.00	19.51	1.28	173.69	13.84	518.31
3.441	0.90	18.66	1.16	173.37	13.03	519.46
3.726	0.78	17.49	1.00	172.97	11.93	520.99
4.023	0.67	16.43	0.87	172.64	10.93	522.36
4.518	0.59	15.79	0.78	172.18	9.92	523.64
5.610	0.52	15.67	0.70	171.39	8.64	525.14
6.934	0.47	15.77	0.65	170.64	7.56	526.37
8.715	0.43	16.06	0.60	169.85	6.55	527.51
12.497	0.37	16.79	0.55	168.63	5.16	529.07
21.923	0.29	18.23	0.49	166.81	3.34	531.08
48.410	0.19	20.09	0.44	164.74	1.49	533.15

TABLE III-3

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 1-CM

Area Ratio	Species Concentration (lb-mol/lb) x 10^4					
	O	H	O_2	H_2	OH	H_2O
1.727	1.78	23.80	2.05	177.94	21.95	507.86
1.941	1.73	24.00	2.04	177.15	20.73	509.15
2.106	1.66	23.78	2.00	176.72	19.94	510.10
2.210	1.57	23.30	1.96	176.21	18.98	511.32
2.414	1.43	22.51	1.78	175.59	17.78	512.94
2.711	1.23	21.16	1.55	174.77	16.09	515.28
3.251	0.92	18.70	1.18	173.64	13.45	518.96
3.631	0.76	17.15	0.97	173.07	11.92	521.07
4.055	0.62	15.76	0.80	172.59	10.55	522.93
4.466	0.59	15.68	0.77	172.21	9.92	523.66
5.431	0.53	15.57	0.70	171.50	8.76	525.01
6.427	0.48	15.63	0.66	170.90	7.88	526.01
9.173	0.42	16.08	0.69	169.68	6.30	527.80
15.594	0.34	17.27	0.52	167.90	4.37	529.95
28.516	0.26	18.83	0.47	166.05	2.62	531.90
46.046	0.19	19.91	0.44	164.87	1.57	533.06

TABLE III-4

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 2-S

Area Ratio	Species Concentration (lb-mol/lb) x 10^4 O	H	O_2	H_2	OH	H_2O
1.124	3.59	32.14	3.59	183.53	32.48	492.50
1.217	3.10	30.93	3.43	182.45	30.69	495.08
1.481	2.42	27.67	2.78	179.73	25.97	501.79
1.772	1.98	25.39	2.34	177.83	22.54	506.55
2.198	1.59	23.32	1.94	175.99	19.17	511.11
2.417	1.45	22.63	1.80	175.30	17.90	512.78
2.717	1.32	21.93	1.66	174.52	16.51	514.61
3.270	1.15	21.18	1.48	173.42	14.60	517.04
3.636	1.08	20.92	1.40	172.84	13.66	518.21
4.125	1.00	20.76	1.32	172.19	12.64	519.46
4.635	0.95	20.73	1.26	171.60	11.79	520.48
5.746	0.87	20.91	1.18	170.57	10.40	522.12
7.160	0.80	21.34	1.11	169.52	9.14	523.58
10.482	0.71	22.48	1.04	167.74	7.20	525.76
16.422	0.61	24.11	0.97	165.70	5.22	527.98
26.911	0.50	25.91	0.92	163.67	3.40	530.01
34.625	0.44	26.73	0.90	162.79	2.64	530.87
41.552	0.41	27.26	0.88	162.23	2.16	531.41

TABLE III-5

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 2-C

Area Ratio	Species Concentration (lb-mol/lb) x 10^4 O	H	O_2	H_2	OH	H_2O
1.123	3.59	32.14	3.59	183.53	32.48	492.50
1.295	3.08	31.15	3.47	181.88	29.66	496.06
1.473	2.79	30.05	3.23	180.39	27.14	499.35
1.722	2.49	28.96	2.97	178.82	24.54	502.77
2.046	2.18	27.69	2.67	177.25	21.94	506.28
2.314	1.91	26.30	2.39	176.15	20.03	509.03
2.621	1.63	24.63	2.07	175.11	18.11	511.86
3.062	1.30	22.27	1.66	173.95	15.72	515.39
3.445	1.07	20.46	1.38	173.20	14.00	517.92
4.073	0.93	19.73	1.22	172.32	12.44	519.93
4.764	0.87	19.79	1.15	171.57	11.37	521.20
6.093	0.79	20.10	1.08	170.43	9.86	522.93
9.425	0.69	21.23	0.98	168.44	7.60	525.49
13.424	0.61	22.44	0.93	166.86	6.00	527.26
18.236	0.55	23.56	0.90	165.54	4.76	528.64
29.216	0.45	25.21	0.85	163.71	3.12	530.46
37.160	0.40	25.96	0.84	162.92	2.43	531.23
43.092	0.38	26.36	0.83	162.48	2.06	531.65

TABLE III-6

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 3-S

Area Ratio	Species Concentration (lb-mol/lb) x 10^4 O	H	O_2	H_2	OH	H_2O
1.083	3.80	33.23	3.80	184.38	33.87	490.48
1.212	3.49	33.24	3.84	183.11	31.80	492.78
1.444	3.17	32.42	3.66	181.16	28.46	496.81
2.008	2.75	31.94	3.34	178.03	23.82	502.49
2.625	2.55	32.46	3.19	175.79	20.89	505.93
3.194	2.44	33.22	3.11	174.22	19.01	508.07
6.714	2.15	37.58	2.99	168.42	12.85	514.77
13.303	1.90	42.12	2.95	163.47	8.13	519.81
22.980	1.72	45.15	2.95	160.33	5.24	522.87
35.282	1.61	46.84	2.96	158.61	3.67	524.53

TABLE III-7

EXACT FLOW SPECIES CONCENTRATIONS FOR RUN 3-CM

Area Ratio	Species Concentration (lb-mol/lb) x 10^4					
	O	H	O_2	H_2	OH	H_2O
1.090	3.80	33.23	3.80	184.38	33.87	490.48
1.281	3.49	33.69	3.86	182.53	31.00	493.53
1.401	3.31	33.08	3.78	181.59	29.20	495.67
1.780	2.61	29.95	3.16	178.90	24.56	502.25
2.024	2.20	27.79	2.72	177.48	22.16	505.95
2.412	1.69	24.65	2.12	175.76	18.99	510.82
2.781	1.34	22.20	1.70	174.58	16.57	514.43
3.275	0.92	18.53	1.17	173.41	13.53	518.96
3.676	0.79	17.45	1.01	172.83	12.18	520.75
4.023	0.69	16.54	0.89	172.42	11.14	522.14
4.612	0.66	16.72	0.85	171.86	10.39	522.99
5.406	0.65	17.33	0.85	171.18	9.69	523.70
8.911	0.62	19.38	0.85	169.05	7.53	525.90
15.692	0.58	21.61	0.85	166.77	5.29	528.18
22.139	0.55	22.81	0.85	165.55	4.12	529.39
27.270	0.53	23.44	0.85	164.91	3.50	530.02
32.679	0.51	23.93	0.85	164.42	3.04	530.50
38.576	0.50	24.33	0.85	164.02	2.66	530.89
41.708	0.50	24.49	0.85	163.86	2.50	531.05

TABLE III-8

EXACT FLOW VALUES FOR RUN 1-S

Area Ratio	Velocity (ft/sec)	Pressure (lb/ft^2)	Temp (Deg R)	Mach Number	Specific Impulse (lb-sec/lb)	Density $\times 10^3$ (lb/ft^3)	Gamma (Frozen)
1.723	8743	7201	5256	1.82	340.1	12.06	1.864
1.834	8964	6497	5180	1.88	344.2	11.04	1.156
2.068	9344	5395	5070	1.98	351.9	9.39	1.146
2.297	9645	4613	4981	2.07	358.1	8.20	1.148
2.645	10020	3754	4862	2.17	366.1	6.85	1.154
2.979	10313	3164	4760	2.26	372.4	5.91	1.159
3.237	10506	2813	4689	2.32	376.7	5.34	1.163
3.662	10780	2364	4581	2.41	382.7	4.60	1.169
3.992	10962	2095	4505	2.48	386.8	4.15	1.173
4.444	11178	1805	4411	2.55	391.6	3.66	1.178
5.306	11514	1414	4254	2.68	399.2	2.97	1.185
7.762	12134	858	3933	2.93	413.3	1.96	1.197
9.458	12455	645	3752	3.08	420.7	1.54	1.203
14.476	13027	365	3404	3.37	434.0	0.96	1.213
19.982	13407	238	3156	3.60	442.9	0.68	1.220
26.050	13690	168	2960	3.78	449.6	0.51	1.226
39.052	14078	99	2679	4.08	458.8	0.33	1.236

TABLE III-9

EXACT FLOW VALUES FOR RUN 1-C

Area Ratio	Velocity (ft/sec)	Pressure (lb/ft^2)	Temp (Deg R)	Mach Mumber	Specific Impulse (lb-sec/lb)	Density x 10^3 (lb/ft^3)	Gamma (Frozen)
1.723	8743	7201	5256	1.82	340.0	12.05	1.577
1.965	9197	5803	5088	1.94	348.7	10.05	1.181
2.234	9589	4747	4937	2.06	356.4	8.48	1.163
2.560	9953	3886	4819	2.16	364.1	7.13	1.141
2.881	10238	3292	4740	2.25	370.4	6.16	1.129
3.253	10512	2786	4666	2.33	376.6	5.31	1.126
3.441	10633	2582	4633	2.37	379.4	4.96	1.127
3.726	10800	2319	4586	2.42	383.2	4.51	1.131
4.023	10956	2092	4538	2.47	386.9	4.12	1.144
4.518	11189	1783	4442	2.55	392.1	3.59	1.184
5.610	11599	1321	4242	2.70	401.3	2.79	1.190
6.934	11966	988	4051	2.85	409.6	2.19	1.196
8.715	12327	725	3850	3.01	417.9	1.69	1.202
12.497	12836	447	3547	3.26	429.7	1.13	1.210
21.923	13510	212	3107	3.65	445.5	0.61	1.222
29.235	13809	145	2898	3.86	452.6	0.45	1.229
48.410	14269	75	2555	4.23	463.4	0.26	1.241

TABLE III-10

EXACT FLOW VALUES FOR RUN 1-CM

Area Ratio	Velocity (ft/sec)	Pressure (lb/ft^2)	Temp (Deg R)	Mach Number	Specific Impulse (lb-sec/lb)	Density x 10^3 (lb/ft^3)	Gamma (Frozen)
1.727	8752	7169	5252	1.82	340.2	12.01	1.201
1.941	9157	5919	5100	1.93	347.9	10.22	1.175
2.106	9354	5363	5032	1.99	351.8	9.39	1.164
2.210	9561	4817	4965	2.05	356.0	8.56	1.154
2.414	9793	4251	4893	2.11	360.9	7.68	1.145
2.711	10087	3602	4808	2.20	367.3	6.64	1.136
3.251	10509	2798	4687	2.33	376.7	5.31	1.132
3.631	10746	2408	4618	2.40	382.1	4.65	1.131
4.055	10973	2074	4546	2.47	387.4	4.08	1.182
4.466	11171	1810	4453	2.54	391.7	3.64	1.185
5.431	11545	1380	4271	2.68	400.1	2.90	1.190
6.427	11843	1096	4118	2.80	406.9	2.39	1.195
9.173	12408	676	3805	3.05	419.8	1.60	1.203
15.594	13122	333	3367	3.42	436.4	0.89	1.215
28.516	13788	150	2915	3.84	452.1	0.46	1.228
46.046	14231	80	2587	4.02	462.5	0.28	1.240

TABLE III-11

EXACT FLOW VALUES FOR RUN 2-S

Area Ratio	Velocity (ft/sec)	Pressure (lb/ft^2)	Temp (Deg R)	Mach Number	Specific Impulse (lb-sec/lb)	Density $\times 10^3$ (lb/ft^3)	Gamma (Frozen)
1.124	6715	15707	5650	1.33	306.0	24.05	1.734
1.217	7250	13119	5534	1.46	313.3	20.57	1.134
1.481	8190	9141	5338	1.68	329.1	14.96	1.138
1.772	8856	6814	5174	1.85	341.8	11.57	1.144
2.198	9525	4891	4980	2.04	355.3	8.67	1.154
2.417	9787	4248	4895	2.11	360.8	8.67	1.158
2.717	10091	3579	4789	2.20	367.2	6.62	1.160
3.270	10531	2743	4620	2.34	376.7	5.27	1.172
3.636	10765	2360	4523	2.42	381.9	4.64	1.177
4.125	11028	1977	4408	2.51	387.7	3.99	1.182
4.635	11257	1680	4300	2.60	392.8	3.48	1.186
5.746	11650	1249	4106	2.75	401.6	2.71	1.193
7.160	12017	925	3911	2.90	410.0	2.11	1.200
10.482	12583	553	3587	3.17	423.0	1.38	1.209
16.422	13154	304	3230	3.48	436.3	0.84	1.219
26.911	13688	158	2866	3.83	448.9	0.49	1.230
34.625	13929	113	2692	4.01	454.6	0.38	1.236
41.552	14091	89	2571	4.15	458.4	0.31	1.241

TABLE III-12

EXACT FLOW VALUES FOR RUN 2-C

Area Ratio	Velocity (ft/sec)	Pressure (lb/ft^2)	Temp (Deg R)	Mach Number	Specific Impulse (lb-sec/lb)	Density $\times 10^3$ (lb/ft^3)	Gamma (Frozen)
1.123	6715	15707	5650	1.33	306.0	24.05	1.530
1.295	7606	11514	5425	1.55	318.6	18.43	1.155
1.473	8195	9102	5272	1.69	328.6	15.04	1.157
1.722	8783	7011	5105	1.84	339.5	12.00	1.160
2.046	9331	5359	4941	1.99	350.4	9.51	1.146
2.314	9674	4468	4846	2.09	357.6	8.11	1.136
2.621	9990	3743	4763	2.18	364.5	6.93	1.127
3.062	10353	3017	4670	2.29	372.7	5.72	1.123
3.445	10610	2571	4602	2.37	378.6	4.97	1.124
4.073	10966	2035	4459	2.49	386.5	4.06	1.185
4.764	11278	1634	4311	2.60	393.4	3.38	1.189
6.093	11725	1163	4086	2.77	403.5	2.54	1.196
9.425	12414	643	3703	3.08	419.2	1.55	1.207
13.424	12894	400	3412	3.33	430.4	1.05	1.214
18.236	13263	266	3173	3.54	439.0	0.75	1.221
29.216	13761	143	2830	3.88	450.7	0.45	1.231
37.160	13988	104	2664	4.05	456.1	0.35	1.237
43.092	14119	85	2565	4.16	459.2	0.30	1.241

TABLE III-13

EXACT FLOW VALUES FOR RUN 3-S

Area Ratio	Velocity (ft/sec)	Pressure (lb/ft^2)	Temp (Deg R)	Mach Number	Specific Impulse (lb-sec/lb)	Density x 10^3 (lb/ft^3)	Gamma (Frozen)
1.083	6404	17277	5699	1.27	302.1	26.17	1.342
1.212	7262	13027	5466	1.47	312.8	20.61	1.169
1.444	8127	9319	5230	1.70	326.7	15.46	1.167
2.008	9289	5415	4849	2.00	348.6	9.73	1.179
2.625	10020	3605	4562	2.22	363.6	6.90	1.188
3.194	10481	2704	4361	2.37	373.3	5.42	1.194
4.163	11028	1853	4101	2.57	385.3	3.95	1.201
6.714	11855	954	3665	2.92	403.8	2.28	1.211
13.303	12787	379	3109	3.41	425.2	1.07	1.225
22.980	13382	183	2712	3.80	439.0	0.59	1.238
35.383	13777	103	2425	4.12	448.3	0.37	1.250

TABLE III-14

EXACT FLOW VALUES FOR RUN 3-CM

Area Ratio	Velocity (ft/sec)	Pressure lb/ft^2)	Temp (Deg R)	Mach Number	Specific Impulse (lb-sec/lb)	Density x 10^3 (lb/ft^3)	Gamma (Frozen)
1.090	6404	17277	5699	1.27	302.1	26.17	1.286
1.281	7575	11605	5365	1.54	317.3	18.71	1.168
1.401	7998	9821	5253	1.65	324.4	16.20	1.154
1.780	8883	6631	5042	1.88	341.1	11.48	1.126
2.024	9273	5472	4958	1.98	349.2	9.67	1.120
2.412	9748	4254	4857	2.11	359.5	7.72	1.112
2.781	10100	3486	4776	2.21	367.3	6.46	1.122
3.275	10465	2801	4711	2.31	375.8	5.30	1.161
3.676	10720	2386	4623	2.39	381.5	4.61	1.143
4.023	10910	2108	4558	2.45	385.8	4.14	1.048
4.612	11192	1737	4419	2.55	392.0	3.52	1.203
5.406	11501	1389	4255	2.67	398.8	2.92	1.205
8.911	12335	698	3779	3.03	417.6	1.65	1.212
15.692	13096	326	3301	3.43	435.2	0.88	1.221
22.139	13488	206	3036	3.68	444.4	0.61	1.227
27.270	13704	157	2884	3.83	449.4	0.49	1.232
32.679	13879	123	2756	3.96	453.6	0.40	1.236
38.576	14032	99	2643	4.08	457.2	0.34	1.240
41.708	14100	89	2590	4.14	458.8	0.31	1.242

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An approximate method is presented which yields the supersonic nozzle profile necessary to keep an expanding high temperature gas mixture approximately in chemical equilibrium. From equilibrium calculations for given chamber conditions, the freeze area ratio is determined by use of a modified Bray criterion. A plot of area ratio versus a function of nozzle geometry defines a limiting nozzle angle beyond which freezing is forecast to occur. This permits an expansion angle at each area ratio to be chosen to keep the flow near equilibrium. The effectiveness of the resulting nozzle profile is evaluated by comparing exact calculations with equilibrium calculations. Contouring is shown to be effective for small nozzles when a correction factor is applied. The hydrogen-oxygen system is used as an example.

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